CFD Analysis of Gasification Process (Downdraft Gasifier)

By

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09MMET04

DEPARTMENT OF MECHANICAL ENGINEERING

INSTITUTE OF TECHNOLOGY

NIRMA UNIVERSITY

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Major Project

Submitted in partial fulfillment of the requirements

For the degree of

Master of Technology in Mechanical Engineering (Thermal Engineering)

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Declaration

This is to certify that

i) The thesis comprises my original work towards the degree of Master of Technology in Mechanical Engineering (Thermal) at Nirma University and has not been submitted elsewhere for a degree.

ii) Due acknowledgement has been made in the text to all other material used.

Patel Keran Dhirubhai

Certificate

This is to certify that the Major Project entitled “CFD Analysis of Gasification Process (Downdraft Gasifier)” submitted by Patel Keran Dhirubhai (09MMET04), towards the partial fulfillment of the requirements for the degree of Master of Technology in Mechanical Engineering (Thermal) of Nirma University of Science and Technology, Ahmedabad is the record of work carried out by him under my supervision and guidance. In my opinion, the submitted work has reached a level required for being accepted for examination. The results embodied in this major project, to the best of my knowledge, haven’t been submitted to any other university or institution for award of any degree or diploma.

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Abstract

Gasification converts carbonaceous pulverized fuels into synthesis gas, a mixture of CO and H_2 that is a raw material for chemicals as well as a fuel for producing electricity. Gasification has the best fuel flexibility of any of the advanced technologies for power production, and current technology has already operated well with biomass and other low-value feed stocks, and with high-ash residues.Gasification produces a much higher concentration of carbon dioxide than direct combustion of coal in air. The higher concentrations of carbon dioxide make carbon capture and storage more economical than it otherwise would be. In view of these, gasification energy combined with Computational Fluid Dynamics (CFD) software has been described in some detail in the following study. The aspect of gasification processes have been investigated with regard to the existing (down-draft) gasifier using simulation in FLUENT software. The project is about the modeling of fluid flow of fuel inside biomass down-draft gasifier using FLUENT software. Using the typical design of down-draft gasifier, the model is produced in 2-Dimension for easier iterations and simulations. The formation of flow pattern, temperature, turbulence, product gas composition, and radiation heat transfer will be investigated.To anticipate the solid's behavior, particle concentration and particle size change due to pyrolysis and surface reactions will be modeled using an Eulerian-Lagrangian approach.

Keywords: - Biomass gasification, CFD, Downdraft gasifier.

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Chapter 1

Introduction

1.1 Gasification - An Introduction

Gasification is a thermo-chemical process that converts carbonaceous materials, such as coal, petroleum, bio-fuel or biomass into carbon monoxide and hydrogen by reacting the raw material, such as house waste, or compost at high temperatures with a controlled amount of oxygen and/or steam. The resulting gas mixture is called synthesis gas or syngas and is itself a fuel. Gasification is a method for extracting energy from many different types of organic materials. The advantage of using gasification is that using the syngas is potentially more efficient than direct combustion of the original fuel because it can be converted at higher temperatures or even in fuel cells, so that the thermodynamic upper limit to the efficiency defined by Carnot's rule is higher or not applicable.

Syngas may be burned directly in internal combustion engines, used to produce methanol and hydrogen, or converted via the Fischer-Tropsch process into synthetic fuel. Gasification can also begin with materials that are not otherwise useful fuels, such as biomass or organic waste. In addition, high-temperature combustion refines out corrosive ash elements such as chloride or potassium, allowing clean gas production from otherwise problematic fuels. Gasification of fossil fuels is currently widely used on industrial scales to generate electricity. However, almost any type of organic material can be used as the raw material for gasification, such as wood, biomass, or even plastic waste. Gasification relies on chemical processes at elevated temperatures greater than 700^oC, which distinguishes it from processes such as anaerobic digestion that produce biogas.

1.1.1 Gasification Approaches

While the characteristics of the product gases from different concepts varies significantly, gasification approaches can be grouped into two general types based on the energy content of the product. The energy content of the gas depends on the approach used to supply heat to drive the gasification reactions.

Most designs use oxygen, either in air or in its separated form, as an oxidizing agent to generate heat by partially combusting the biomass feedstock. When heat is supplied by partial oxidation with air (air-blown gasification), nitrogen in the air dilutes the product. The resulting gas is classified as a low-energy gas and has a heating value of approximately 2.5- 8.0 MJ/Nm^3. Low-energy gasifiers are best used in situations where the heat content of the gas is not a critical issue such as co-firing applications, district heating systems, and many electric generation systems. Medium-energy gases can be produced using pure oxygen instead of air as the oxidizing agent to provide heat for the gasification. The use of separated oxygen eliminates the nitrogen diluent, and a medium-energy gas (10-20 MJ/Nm^3) can be produced.

In the absence of oxygen, medium-energy gases can also be produced by pyrolytic gasification by using a reactor where heat for the gasification is provided from an external source (indirectly-fired gasification). In these gasifiers, heat is provided using methods such as heat exchangers and circulating the hot bed material. Medium-energy gasifiers are appropriate for situations where a higher energy-content gas is desired. The synthesis of liquid fuels requires the use of medium-energy gasifiers since these systems cannot effectively deal with the dilution of the product by nitrogen that occurs in air-blown systems.

1.1.2 Chemistry

The substance of a solid fuel is usually composed of the elements carbon, hydrogen and oxygen. In the gasifiers considered, the biomass is heated by combustion. Four different processes can be distinguished in gasification: drying, pyrolysis, oxidation and reduction.

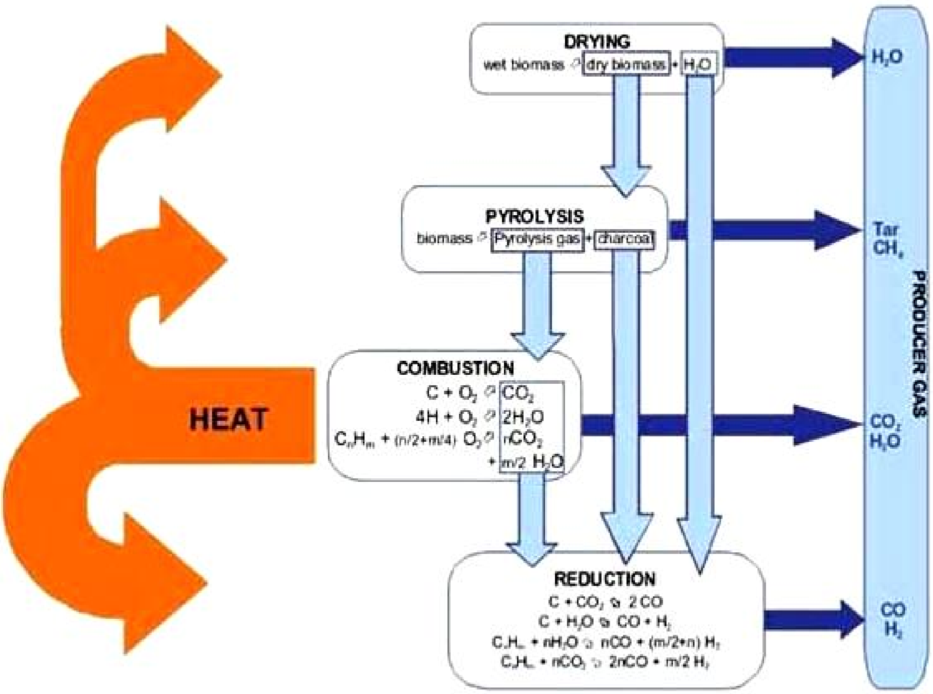

Figure 1.1: Chemistry of Biomass Gasification

1.1.3 Direct Gasification

In direct gasification, Oxygen or Air is used as blast. Gasification can be accomplished by using the principal of partial oxidation. In this case exothermic gasification occurs by supplying sub-stoichiometric blast to the process. The equivalence ratio (ER) is the amount of oxidant supplied relative to the stoichiometric requirement. Optimum gasification efficiency occurs near an equivalence ratio of 0.26 in purely direct biomass gasification. In practical reality, incomplete conversion will occur due to kinetic limitations of volatile matter conversion and heat and mass transfer limitations of fixed carbon conversion. These affects relate to reactor design constraints and system configuration effects. The amount of tar in the generated gas often depends on reactor design. Minimizing tar with creative equipment design is a principal goal for gasification engineers.

1.1.4 Indirect Gasification

Indirect gasification is accomplished using steam as an oxidant. However, steam reforming of biomass is endothermic and often heat transfer limited. Endothermic gasification generates more methane than direct gasification per volume of gas, so the energy density may be higher. The thermal input required for steam reforming of biomass means that some clever method of high rate heat transfer must be devised. Steam gasification is thermodynamically more efficient than direct gasification, but practical heat transfer limitations and thermodynamic availability requirements for high temperature heat exchange often makes reality a bit different.

1.2 Types of Gasifiers

1.2.1 The Updraft Gasifier

Updraft gasifiers are mainly divided in to two parts.

- Updraft charcoal gasifier
- Counter-current fixed bed updraft gasifier

Updraft charcoal Gasifiers were first to be developed for vehicle operation. They are suitable only for low tar fuels such as charcoal and coke.

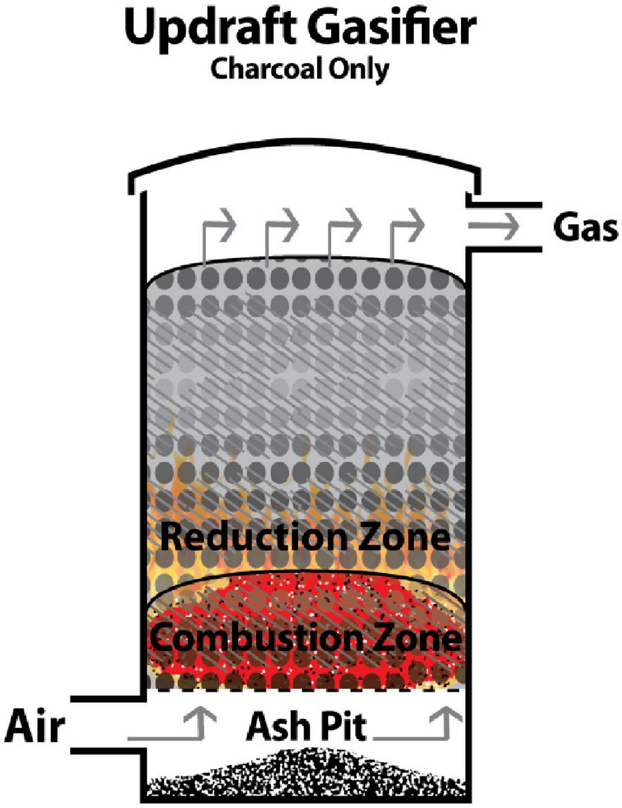

Figure 1.2: Updraft Gasifier (Charcoal only)

Air from below the grate (sometimes accompanied by steam), is blown up through the fuel pile. Since the flow of fuel is downward, toward the grate, and since the flow of air is upward, up through the fuel pile, this type of gasifier is also called a“counter-flow” gasifier. High temperatures at the air inlet can easily cause slagging or destruction of the grate, and often some stream or CO, is added to the inlet air to moderate the grate temperature. Charcoal updraft Gasifiers are characterized by comparatively long starting times and poor response because of the large thermal mass of the hearth and fuel zone.

As the wood waste works its way down to the grate it dries, its volatiles are pyrolyzed and its fixed carbon (also known as "char") is converted to carbon monoxide. In the process some of the char is completely oxidized to liberate the heat needed for evaporation and pyrolyzation. The carbon dioxide, so formed, is usually reduced to carbon monoxide as it continues its way up through additional layers of char to the top of the fuel pile. The producer gas leaving the gasifier is at a low temperature.

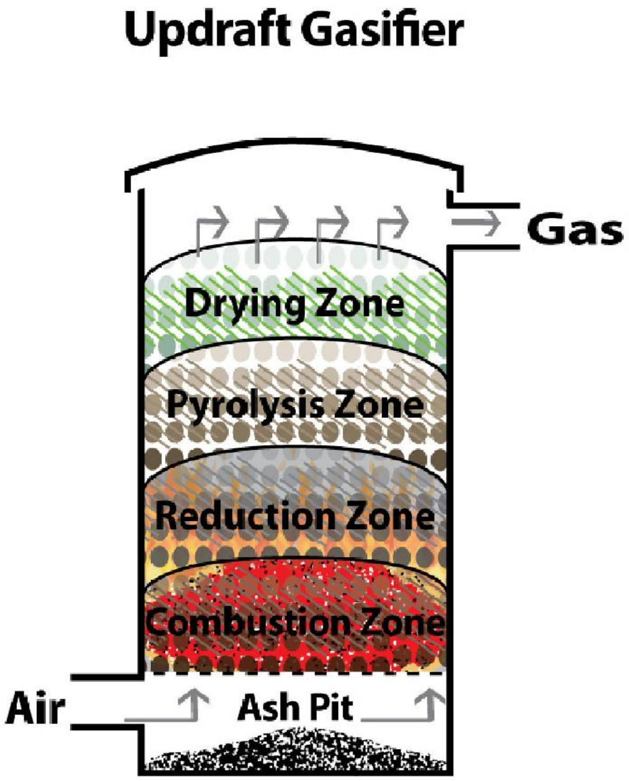

Figure 1.3: Counter-current fixed bed Gasifier

The counter-current fixed bed ("up draft") gasifier consists of a fixed bed of carbonaceous fuel (e.g. coal or biomass) through which the "Gasification agent" (steam, oxygen and/or air) flows in counter-current configuration. The ash is either removed dry or as a slag. The nature of the gasifier means that the fuel must have high mechanical strength and must ideally be non-caking so that it will form a permeable bed, although recent developments have reduced these restrictions to some extent. The throughput for this type of gasifier is relatively low. Thermal efficiency is high as the gas exit temperatures are relatively low.

Updraft Gasifiers are thermally efficient because the ascending gases pyrolyzed and dry the incoming biomass, transferring heat so that the exiting gases leave very cool.

1.2.2 The Cross draft Gasifier

Air enters at high velocity through a single nozzle, induces substantial circulation, and flows across the bed of fuel and char. This produces very high temperatures in very small volume and results in production of a low tar-gas, permitting rapid adjustment to engine load changes. The fuel and ash serve as insulation for the walls of the gasifier, permitting mild steel construction for all parts except the nozzles and grates, which may require refractory alloys or some cooling. Air cooled or water cooled nozzles are often required. The high temperatures reached require a low-ash fuel to prevent slagging.

The disadvantages such as high exit gas temperature, Poor CO_2 reduction and high gas velocity are the consequence of the design. unlike downdraft and updraft gasifiers, the ash bin, fire and reduction zone in crossdraft gasifiers are separated. This design characteristics limit the type of fuel for operation to low ash fuels such as wood, charcoal, and coke. The load following ability of crossdraft gasifier is quite good due to concentrated partial zones which operates at temperatures up to 2000^oC Start up time (5-10 minutes) is much faster than that of downdraft and updraft units. The relatively higher temperature in crossdraft gasifier has an obvious effect on gas composition such as high carbon monoxide, and low hydrogen and methane content when dry fuel such as charcoal is used. Crossdraft gasifier operates well on dry blast and dry fuel.

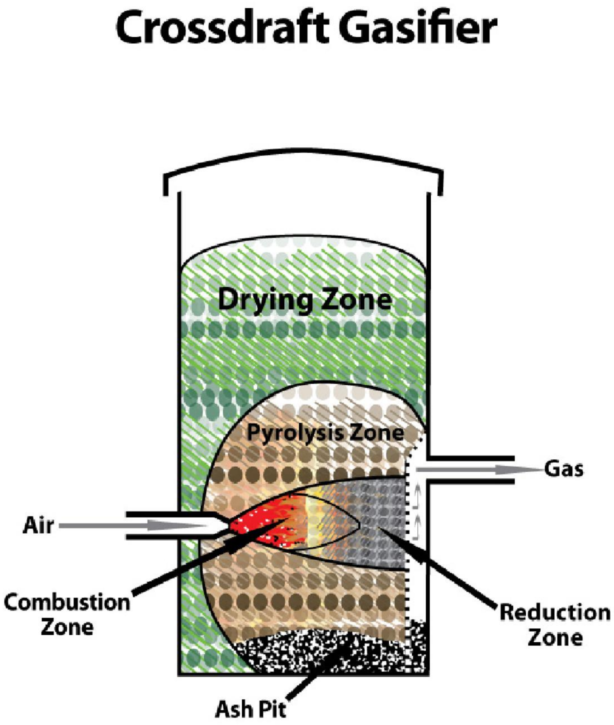

Figure 1.4: Crossdraft Gasifier

The cross draft gasifier is generally considered suitable only for low-tar fuels. Some success is observed with un-pyrolyzed biomass, but the nozzle-to-grate spacing is critical. Cross draft Gasifiers have the fastest response time and the smallest thermal mass of any gas producers because there is a minimum inventory of hot charcoal. In one design, a down-draft gasifier could be operated in a cross draft scheme during start up in order to minimize the start up time.

1.2.3 The Down-draft Gasifier

Introduction

The constricted hearth, down-draft gasifier is sometimes called the 'Imbert' gasifier after its inventor, Jacques Imbert; although, it has been commercially manufactured under various names. These units cost about dollar 1500 (1985 evaluation) each. However, after World War II began in 1939, it took six to eight months before factory-made gasifiers were generally available.

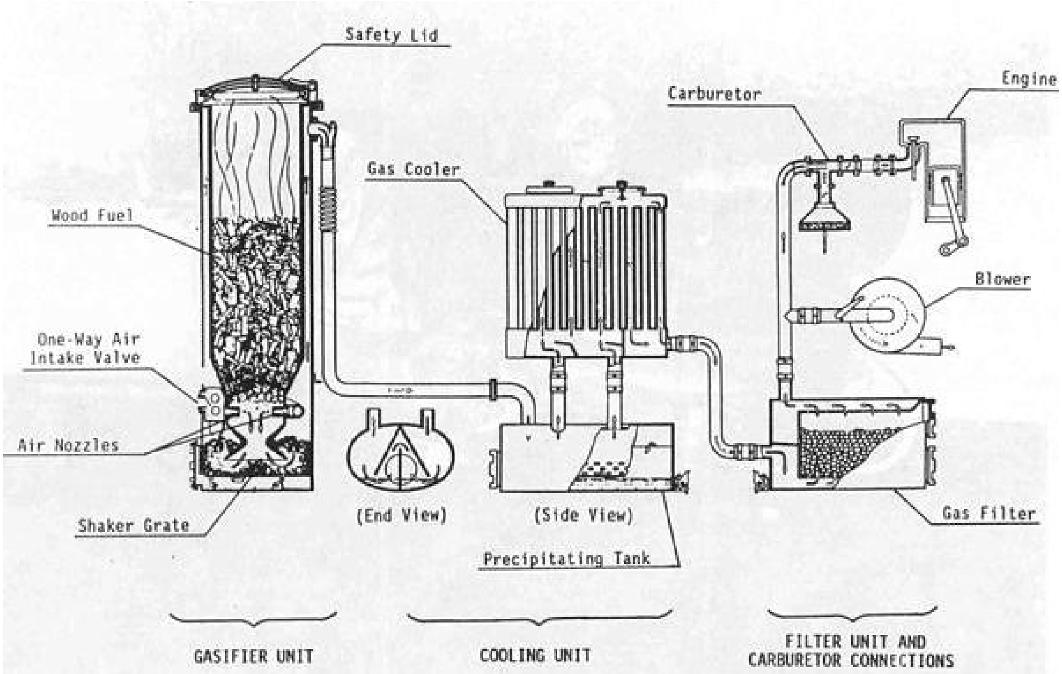

Figure 1.5: Imbert Downdraft Gasifier

In Figure 1.5, the upper cylindrical portion of the gasifier unit is simply a storage bin or hopper for wood chips or other biomass fuel. During operation, this chamber is filled every few hours as needed. The spring-loaded, airtight cover must be opened to refill the fuel hopper; it must remain closed and sealed during gasifier operation. The spring permits the cover to function as a safety valve because it will open in case of any excessive internal gas pressure. About one-third of the way up from the bottom of the gasifier unit, there is a set of radially directed air nozzles; these allow air to be injected into the wood as it moves downward to be gasified. The gas is introduced into the engine and consumed a few seconds after it is made. This gasification method is called “producer gas generation” because no storage system is used; only that amount of gas demanded by the engine is produced. When the engine is shut off, the production of gas stops. During normal operation, the incoming air burns and pyrolyzes some of the wood, most of the tars and oils, and some of the charcoal that fills the constricted area below the nozzles. Most of the fuel mass is converted to gas within this combustion zone. The Imbert gasifier is, in many ways, self-adjusting. If there is insufficient charcoal at the air nozzles, more wood is burned and pyrolyzed to make more charcoal. If too much charcoal forms, then the charcoal level rises above the nozzles, and the incoming air burns the charcoal. Thus, the combustion zone is maintained very close to the nozzles.

Below this combustion zone, the resulting hot combustion gases - carbon dioxide (CO_2) and water vapor (H_2O) - pass into the hot charcoal where they are chemically reduced to combustible fuel gases: carbon monoxide (CO) and hydrogen ($\mathrm{H_2}$). The hearth constriction causes all gases to pass through the reaction zone, thus giving maximum mixing and minimum heat loss. The highest temperatures are reached in this region. The charcoal is supported by a movable grate which can be shaken at intervals. Usually, wood contains less than 1% ash (by weight). However, as the charcoal is consumed, it eventually collapses to form a powdery charcoal/ash mixture which may represent 2 to 10% (by weight) of the total fuel mass. The cooling unit required for the imbert gasifier consists of water filled precipitating tank and an automotive radiator type gas cooler. A second filter unit, containing a fine mesh filtration material, is used to remove the last traces of any ash or dust that may have survived passage through the cooling unit. Once out of the filter unit, the wood gas is mixed with air in the vehicle's carburettor and is then introduced directly into the engine's intake manifold.

Disadvantages of imbert design

Although the imbert gasifier has been the prototype down-draft gasifier, it has a number of disadvantages. The constricted hearth design seriously limits the range of wood fuel shapes that can be successfully gasified without expensive cubing or pelletizing pre-treatment. It is this limitation that makes the imbert gasifier less flexible for emergency use. The imbert gasifier requires a high grade, usually hard wood, fuel, generally at least 2 cm along the smallest dimension with no more than 20% moisture. The imbert design cannot be scaled up to larger sizes because the air enters at the sides and is incapable of penetrating the large diameter fuel bed unless the fuel size is increased proportionally. The tar travel, while low (usually 5000 ppm), is still high enough to require extensive scrubbing and disposal procedures. Unfortunately, there is no overall theory of operation for imbert gasifiers that would permit sizing the gasifier for the fuels other than hardwood blocks. The geometry and flow of fuel and air are quite complex, making any attempts to model the gasifier very difficult tasks indeed.

- The Stratified Down-draft Gasifier

This simplified design employs a balanced, negative-pressure concept in which the old type of sealed fuel hopper is no longer necessary. A closure is only used to preserve the fuel when the engine is stopped. This new technology has several popular names, including ‘stratified down-draft gasification’ and ‘open top gasification’. Two years of laboratory and field testing have indicated that such simple, inexpensive gasifiers can be built from existing hardware and will perform very well as emergency units.

A schematic diagram of the stratified, down-draft gasifier is shown in Figure 1.6.During operation of this gasifier, air passes uniformly downward through four zones, hence the name ‘stratified’:

a. The uppermost zone contains un-reacted fuel through which air and oxygen enter. This region serves the same function as the fuel hopper in the imbert design.

b. In the second zone, the wood fuel reacts with oxygen during pyrolysis. Most of the volatile components of the fuel are burned in this zone and provide heat for continued pyrolysis reactions. At the bottom of this zone, all of the available

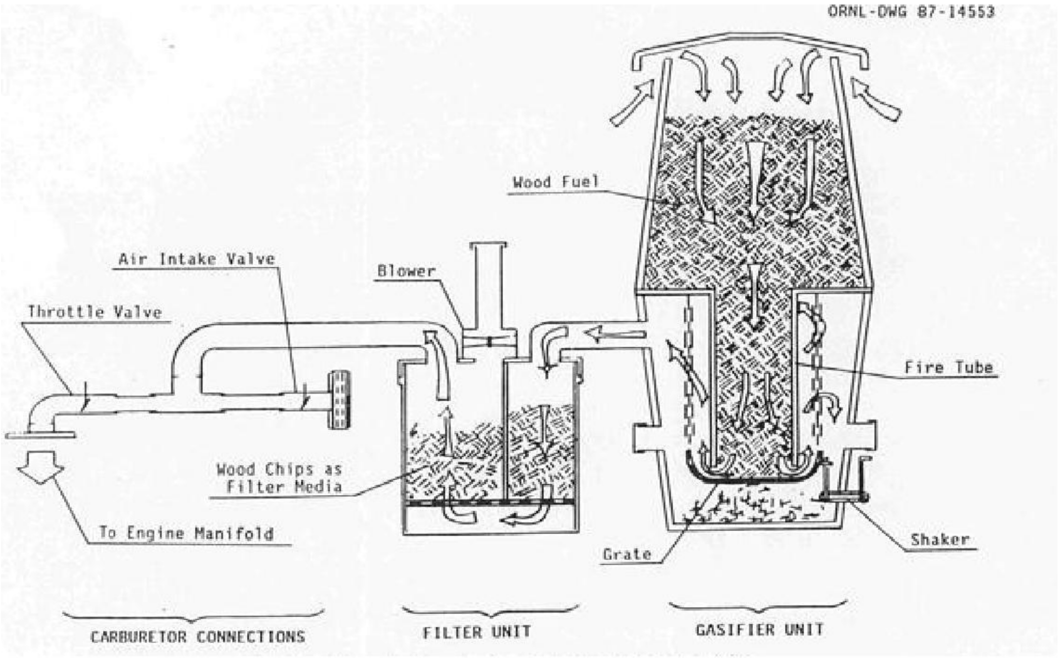

Figure 1.6: Stratified Downdraft Gasifier

oxygen from the air base completely reacted. The open top design ensures uniform access of air to the pyrolysis region.

c. The third zone is made up of charcoal from the second zone. Hot combustion gases from the pyrolysis region react with the charcoal to convert the carbon dioxide and water vapor into carbon monoxide and hydrogen.

d. The inert char and ash, which constitute the fourth zone, are normally too cool to cause further reactions; however, since the fourth zone is available to absorb heat or oxygen as conditions change, it serves both as a buffer and as a charcoal storage region. Below this zone is the grate. The presence of char and ash serves to protect the grate from excessive temperatures.

The stratified, down-draft design has a number of advantages over the imbert gasifier. The open top permits fuel to be fed more easily and allows easy access. The cylindrical shape is easy to fabricate and permits continuous flow of fuel. No special fuel shape or pre-treatment is necessary; any blocky fuel can be used. The foremost question about the operation of the stratified, down-draft gasifier concerns char and ash removal. As the charcoal reacts with the combustion gases, it eventually reaches a very low density and breaks up into a dust containing all of the ash as well as a percentage of the original carbon. This dust may be partially carried away by the gas; however, it might eventually begin to plug the gasifier, and so it must be removed by shaking or agitation. Both the imbert gasifiers and the stratified concept have a provision for shaking the grate; when they are used to power vehicles, they are automatically shaken by the vehicle's motion.

1.3 CFD Modeling of Gasifier

CFD modeling techniques are becoming widespread in the thermochemical conversion area. Researchers have been using CFD to simulate and analyze the performance of thermochemical conversion equipment such as fluidized bed gasifiers, fixed bed gasifiers, combustion furnaces, firing boilers, rotating cones and rotary kilns. CFD programs predict not only fluid flow behavior, but also heat and mass transfer, chemical reactions (e.g. devolatilization, combustion), phase changes (e.g. vapor in drying, melting in slagging), and mechanical movement (e.g. rotating cone reactor). Compared to the experimental data, CFD model results are capable of predicting qualitative information and in many cases accurate quantitative information. CFD modeling has established itself as a powerful tool for the development of new ideas and technologies.

However, CFD modeling for thermochemical conversion still face significant challenges due to the complexity of the lignite feedstock and the thermochemical process. Lignite is a mixture of lignin, minor amounts of other organics with proportion and chemical structure affected by variety. Inorganic ash is also part of the biomass composition. The complex structure makes lignite compositions pyrolyze or degrade at different rates by different mechanisms and affect each other during thermochemical process.How to deal with or simplify the complex process is a key point for the CFD simulation model. Many studies have been done on the biomass pyrolysis kinetics and the transfer and tracking of the feedstock particles, which have applied to CFD modeling and made good achievements. Simulations on reactor design, pyrolysis process, combustion systems, particle deposit and pollutant release have been performed with CFD packages.

1.4 Organization of Thesis

The thesis has been divided in to six chapters.First Chapter is all about the basics of gasification, gasification approaches and types of gasifiers.
In the Second chapter, history of the gasification process, review of the present work as well as aim and objectives of the study are included.
Third chapter includes basics about CFD, discretization methods, theoretical considerations in CFD and solution methodology.
Fourth chapter deals with modeling and simulation of down-draft gasifier.Boundary conditions, initial conditions and model parameters settings are also included in the same chapter.
Chapter five contains results which are derived after the simulation on CFD is been carried out.
Chapter six is all about the conclusion and the future work.
Last but not the least,Bibliography is also included in the end of the thesis.

Chapter 2

Literature Review

2.1 History of gasification process

During World War II over a million gasifiers were built for the civilian sector while the military used up all the gasoline. Now that world oil supplies are being depleted and global warming is perceived as a threat to our environment, there is renewed interest in gas from biomass. "Wood gas" is the name for various gases that can be easily made from wood or biomass. Various forms are: Synthesis gas, typically 40% hydrogen (H_2), 40% carbon monoxide (CO), 3% methane (CH_4), and 17% carbon dioxide (CO_2); producer gas, made by gasifying biomass with air; pyrolysis or similar to synthesis gas, but including lots of water and tar are accompanied by production of 10-30% of charcoal. The history of gasification dates back to seventeenth century. Since the conception of idea, gasification has passed through several phases of development. Year wise development of the technology is given below.

1669 Thomas Shirley conducted crude experiments with carborated hydrogen.
1699 Dean Clayton obtained coal gas from pyrolytic experiment.
1788 Robert Gardner obtained the first patent with regard to gasification.
1792 First confirmed use of producer gas reported, Murdoc used the gas generated

from coal to light a room in his house. Since then, for many years coal gas was used for cooking and heating.

1801 Lampodium proved the possibility of using waste gases escaping from charring of wood.

1804 Fourcroy found the water gas by reaction of water with a hot carbon.

1812 developed first gas producer which uses oil as fuel.

1840 First commercially used gasifier was built in France.

1861 Real breakthrough in technology with introduction of Siemens gasifier. This gasifier is considered to be first successful unit.

1878 Gasifiers were successfully used with engines for power generation.

1900 First 600 hp gasifier was exhibited in Paris. Thereafter, larger engines up to 5400 hp were put into service.

1901 J.W. Parker run a passenger vehicle with producer gas.

In the period 1901-1920, many gasifier-engine systems were sold and used for power and electricity generation.

1930 Nazi Germany accelerated effort to convert existing vehicles to producer gas drive as part of plan for national security and independence from imported oil.

1930 Began development for small automotive and portable gas producer. British and French Government felt that automotive charcoal gas producer is more suitable for their colonies where supply of gasoline was scarce and wood that could charred to charcoal was readily available.

1939 About 2, 50,000 vehicles were registered in the Sweden. Out of them, 90 % were converted to producer gas drive. Almost all of the 20,000 tractors were operated on producer gas. 40% of the fuel used was wood and remainder charcoal.

After 1945 after end of Second World War, with plentiful gasoline and diesel available at cheap cost, gasification technology lost glory and importance.

1950-1970 During these decades, gasification was “Forgotten Technology”. Many governments in Europe to felt that consumption of wood at the prevailing rate will reduce the forest, creating several environmental problems.

After 1970 the year 1970s brought a renewed interest in the technology for power generation at small scale. Since then work is also concentrated to use fuels other than wood and charcoal.
1970 IGCC Studies by U.S. DOE.
1970 Gasification of Oil for Hydrogen in the Refining Industry.
1983 Gasification of Coal to Chemicals Plant (Eastman Chemical).
1984 First Coal IGCC Demonstration (Cool water Plant).
1990 First Non-Recourse Project Financed Oil IGCC Projects (Italy).
1993 First Natural Gas Gasification F-T Project (Shell Bintulu).
1994 NUON/Demkolec's 253 MWe Buggenum Plant Begins Operation.
1995 PSI Walbash, Indiana Coal IGCC Begins Operation (DOE CCT IV).
1996 Tampa Electric Polk Coal IGCC Begins Operation (DOE CCT III).
1997 First Oil Hydrogen/IGCC Plant Begin Operations (Shell Pernis).
1998 ELCOGAS 298 MWe Puertollano Plant.
2002 IGCC is now an Accepted Refinery and Coal Plant Option.

2.2 Applications of Gasification

- **Producer gas**

  It can be obtained from gasification and employed in thermal application or for mechanical / electrical power generation. Like any other gaseous fuel, producer gas affords much better control over power levels when compared to solid fuel. This also paves the way for more efficient and cleaner operation.

- **Thermal Applications**

  For thermal applications, gasifiers are a good option as they can be retrofitted with existing devices such as ovens, furnaces, boilers, etc. Thermal energy of the order of 4.5 to 5.0 MJ is released by burning 1 cubic meter of producer gas in the burner. Flame temperatures in the range of 1200°c can be obtained by optimal air preheating and premixing of air with gas. A few of the devices which could be retrofitted with gasifiers are furnaces for melting non-ferrous metals and for heat treatment, tea dryers, ceramic kilns, boilers for process steam and thermal fluid heaters.

- **Power Generation**

  A diesel engine can be operated on dual fuel mode using producer gas. Diesel substitution of over 80% at high loads and 70 - 80% under normal load variations can be achieved. The mechanical energy thus derived can be used either for driving water pumps for irrigation or for coupling with an alternator for electrical power generation. Alternatively, a gas engine can be operated with producer gas on 100% gas mode with suitably modified air / fuel mixing and control system. This application places constraints on the tar content in the producer as high levels of tar content can damage and reduce the efficiency of the engine.

  Theoretically, almost all kinds of solid wastes and coals with moisture content of 5- 30% can be gasified. However, not every biomass fuel can lead to the successful gasification. Most of the development work is carried out with common fuels such as coal, charcoal and wood. It was recognized that fuel properties such as surface, size, shape as well as moisture content, volatile matter and carbon content influence gasification.

2.3 Chemical Kinetics of Gasification

During the process of coal gasification, various chemical and physical processes occur simultaneously. It is necessary to model the kinetics of these systems to conduct an accurate simulation of a gasifier. The following processes are the major phenomena which occur:

a. **Pre Heating**

This involves pre-heating of the fuel and air for better gasification.

b. **Drying**

Drying is first major process occurring inside the gasifier. It takes place at nearly 50-150 °c where all the moisture in the coal is converted into steam. The steam helps in reduction further down the system. The rate of drying is affected by numerous factors such as temperature, velocity of the feed, moisture content, external surface area and diffusivity.

c. **Devolatilization**

In the devolatilization (pyrolysis) zone, the volatile components which are present in the coal, including various aromatic and tarry compounds, get vaporized and the remaining coal gets converted into char. Typically, pyrolysis occurs at 200-800 °c and produces char, carbon monoxide, carbon dioxide, water vapor, methane, other higher hydrocarbons, pyroligneous acids and tars. Pyrolysis is affected by various factors such as pyrolysis temperature, rate of heating, physical & chemical characteristics of feed and presence of catalytic compounds.

d. **Gasification**

In the gasification process, primarily the char and other solid/liquid organic compounds gets reduced and oxidized to form various gases which make up the output gas. This is one of the key processes in the process of Biomass gasification and optimization of this process can help in increasing the calorific value of the fuel while at the same time reducing the amount of tar content in the fuel.

2.4 Producer Gas

Producer gas is the mixture of combustible and non-combustible gases as shown in Table I . The quantity of gases constituents of producer gas depends upon the type of fuel and operating condition.

Table I: Producer Gas and its Constituents

Constituents	%
CO	10-30
CO_2	5-15
H_2	10-20
CH_4	2-5
N_2	45-60
H_2O	6-8

Table II: Density and Heating Value of different Gases

Gas Type	Density	Heating Value
	Kg/m^3	MJ/m^3
Carbon Monoxide	1.2	13
Carbon Dioxide	2.0	0
Hydrogen	0.1	11
Methane	0.8	35
Nitrogen	1.3	0
Producer Gas	1.2	5

The heating value of producer gas vary from 4.5 to 6 MJ/m^3. Heating value of producer gas is depends on heating value and density of its constituent as shown in Table II. Carbon monoxide is produced from the reduction of carbon dioxide and its quantity varies from 10 to 30 % by volume basis. Although carbon monoxide posses higher octane number of 106, its ignition speed is low. This gas is toxic in nature. Hence, human operator needs to be careful while handling gas. Hydrogen is also a product of reduction process in the gasifier. Hydrogen posses the octane number of 60-66 and it increases the ignition ability of producer gas. Methane and hydrogen are responsible for higher heating value of producer gas. Amount of methane present in producer gas is very less (up to 5 %). Carbon dioxide and nitrogen are non-combustible gases present in the producer gas.

Compared to other gas constituents, producer gas contains highest amount (45-60 %) of nitrogen. The amount of carbon dioxide varies from 5 to 15 %. Higher percentage of carbon dioxide indicates incomplete reduction. Water vapors in the producer gas occur due to moisture content of air introduced during oxidation process, injection of steam in gasifier or moisture content of biomass fuels.

2.5 Concise project definition: motivation for current work

Product gas from biomass gasification can be used in many applications such as in industrial or residential area. Most of this energy production applications are decentralized and coupled with gas turbine or engine and also boiler. A solid fuel fired for gas turbine combustor should have a high intensity and produce complete carbon utilization. Besides that it should maintain fine fly ash particle size and also have low pressure drop and good turndown.

The technologies for primary conversion of biomass for electricity combustion involve these processes which are direct combustion, gasification and pyrolysis. In direct combustion, the oxidation of biomass takes place with excess air. It will produce hot flue gases which are used to produce steam in the heat exchange sections of boilers. The steams produce from the combustion is used to produce electricity in a Rankine Cycle. Normally, only electricity is produced in a condensing steam cycle while electricity and steam are co generated in an extracting steam cycle.

As for gasification cycles, biomass is partially oxidized by stoichiometric amounts of oxygen normally with the present of steam. Then it will provide energy for thermal conversion of the remaining biomass to gases and organic vapors. For power production, the cleaned gasification product gases will be led directly to a boiler or the combustion section of an industrial or turbine.

As for pyrolysis, it uses indirect heat to convert solid organic materials, into gases and liquids. Conversion is carried out in a reaction chamber where air (oxygen) is excluded. The material within the reaction chamber is heated to temperatures of between 400 - 800^{o}C usually by combusting a portion of the gaseous or liquid products. The resultant products of the pyrolysis process always include gas, liquid and solid char. Operating conditions and reactor design can be selected to control the relative proportions produced from the process.

According to Richard et al (1996)[19] in indirect gasification cycles external heat source is used instead of oxygen, that provides the energy for high-temperature steam gasification of the organic fraction of biomass to vapors and gases. Therefore, temperature is very important as the sources of the combustion engine from the product gas.

2.6 Review of present work in gasification

Ratnadhariya J. K. and Channiwala S. A.[12] have done three zone equilibrium and kinetic free modeling of biomass gasifier. This model clearly provides an operating range of equivalence ratio and moisture content for the woody biomass materials. Further, this model facilitates the prediction of the maximum temperature in the oxidation zone of gasifier, which provides useful information for the design of the gasifier and selection of the material for the construction. The merits of the model lies in the fact that it is capable of handling predictions for all category of biomass materials with a wide operating range of equivalence ratio and moisture content in all of the three principal zones of the gasifier.

Basically for biomass gasifier, the processes involved are gasification and pyrolysis processes. Gasification is a partial oxidation process in which organic materials in biomass are converted to a mixture of gas phase, energetic compounds, such as carbon monoxide, hydrogen and methane. Carbon is rejected to form char which is oxidized within the process to produce additional gases, an ash residue and the heat energy necessary to drive the reactions. It is archived by thermally degrading organic materials in the absence of adequate air to support full combustion.

Gao Ningbo and Li Aimin [7] have simulated the behavior of a global fixed bed biomass gasification reactor. The numerical method applied is a Runge-Kutta fourth order method for solution of the pyrolysis zone model and finite differences for the reduction zone model to solve numerically the coupled ordinary differential equations. Simulations are performed for the varying pyrolysis temperature with a heating rate of 25 K/min and constant temperature of 1400 K as the initial reduction zone temperature at the same time.

Watanabe H. and Otaka M. [10]have modeled coal gasification reaction, and prediction of gasification performance for an entrained flow coal gasifier. The coal gasification model suggested in this paper is composed of a pyrolysis model, char gasification model, and gas phase reaction model. A numerical simulation with the coal gasification model is performed on the CRIEPI 2 tons/day (T/D) research scale coal gasifier. Influence of the air ratio on gasification performance, such as a per pass carbon conversion efficiency, amount of product char, a heating value of the product gas, and cold gas efficiency is presented with regard to the 2 T/D gasifier. Gas temperature distribution and product gas composition are also presented. A comparison between the calculation and experimental data shows that most features of the gasification performance were identified accurately by the numerical simulation, confirming the validity of the current model.

Melgar Andres, Perez Juan F., Laget Hannes, Laget Hannes, Horillo Alfonso[15] discussed a mathematical model for the thermochemical processes in a down-draft biomass gasifier. The model combines the chemical equilibrium and the thermodynamic equilibrium of the global reaction, predicting the final composition of the producer gas as well as its reaction temperature. This work includes a parametric study of the influence of the gasifying relative fuel/air ratio and the moisture content of the biomass on the characteristics of the process and the producer gas composition. The model helps to predict the behavior of different biomass types and is a useful tool for optimizing the design and operation of down-draft biomass gasifiers.

Jun Liu Xiang, Rong Zhang Wu and Jun Park Tae [13]have done coal gasification processes in a slurry-feed-type entrained-flow gasifier. Novel simulation methods as well as numerical results are presented. They used the vorticity-stream function method to study the characteristics of gas flow and a scalar potential function is introduced to model the mass source terms. The random trajectory model is employed to describe the behavior of slurry-coal droplets. Very detailed results regarding the impact of the O_2/coal ratio on the distribution of velocity, temperature and concentration are obtained. Simulation results show that the methods are feasible and can be used to study a two-phase reacting flow efficiently.

BERMUDEZ A., FERRIN J. L. and LINAN A. [3]contribute to the mathematical modeling of the combustion of coal particles in pulverized coal furnaces. The model dealt with the gas and solid phases of the flow. For the coal particles a Lagrangian description is used, taking into account the simultaneous processes of moisture evaporation and devolatilization together with the heterogeneous gasification reactions of the char. An Eulerian description will be used for the distributions of temperature and concentrations in the gas phase, with the effect of the particles represented by volumetric sources of heat, mass and momentum. The gas phase oxidation reactions of the volatile, H_2 and CO will be modeled sing the assumption of infinitely fast rates; the Burke-Schumann analysis will be generalized to account for the competition for oxygen of CO, H_2 and the volatile. These reactions may occur, in the form of group combustion, in a gaseous thin diffusion flame separating a region without oxygen, where the coal particles generate volatile, H_2 and CO, from a region with oxygen, where the reactions may occur inside the particles or, outside, in diffusion flames surrounding the individual particles, even though for small particle sizes the gas phase reactions can be considered as frozen near the particles. The analysis will provide relations for the volumetric sources appearing in the gas phase description, and for the rates that determine the evolution of the temperature and mass content of moisture, volatile and char in the particles.

Noorhelinahani Abu Bakar [2]has investigated the aspect of biomass gasifier with regard to the potential of designing future gasifier using simulation in FLUENT software. The project is about the modeling of fluid flow of biomass fuel inside biomass down-draft gasifier using FLUENT software. Using the typical design of gasifier, the model is produced in 2 Dimensional for easier iterations and simulations. Two types of gasifier are measured; pressurized and atmospheric gasifier. The gasifier's model is set to have initial temperature at 800^oCfor both types of gasifier and 5.0 MPa for pressurized gasifier. After iterations in FLUENT software with first-order discretization, the results obtained are convergent and show that using second-order discretization is not suitable for 2-Dimensional model. Finally, future investigations are also suggested in this study for more accurate result using computational fluid dynamic (CFD) software.

Wang Yiqun and Yan Lifeng [22] did CFD modeling on biomass thermochemical processes.Computational fluid dynamics (CFD) modeling applications on biomass thermochemical processes help to optimize the design and operation of thermochemical reactors.This paper introduces the fundamentals involved in developing a CFD solution. Mathematical equations governing the fluid flow, heat and mass transfer and chemical reactions in thermochemical systems are described and sub-models for individual processes are presented. It provides a review of various applications of CFD in the biomass thermochemical process field.

Syred Nick, Kurniawan Katon, Griffiths Tony, Gralton Tom, Ray Ruby [21] made the codes for CFD. Commercial CFD codes such as Fluent are well developed and have well proven routines for lagrangian tracking of burning particles through complex flow fields.Existing models for solid fuel combustion can be adjusted to predict the initial flow field aerodynamics, sometimes the temperature, but fall down when particles have to be followed completely through a system.This is manifested with cyclone combustors and gasifiers via enhanced retention of burning particles in centrifugal force fields, which can only be resolved by changes in the particle size distribution and thus fragmentation as the particle gasify or burn. The difficulties of incorporating models of fragmentation and flow in CFD codes such as Fluent are discussed.

It is concluded from the paper that the model so implemented shows improved prediction in many difficult areas, but still needs development to better reflect actual fragmentation conditions in different experimental systems.

Fletcher D.F., Haynes B.S., Christo F.C., Joseph S.D.[6] developed a model to simulate the flow and reaction in an entrained ow biomass gasifier. The model is based on the CFX package and represents a powerful tool which can be used in gasifier design and analysis. Biomass particulate is modeled via a Lagrangian approach as it enters the gasifier, releases its volatile and finally undergoes gasification.The model provides detailed information on the gas composition and temperature at the outlet and allows different operating scenarios to be examined in an efficient manner.

Papadikis K., Gub S.,Bridgwater A.V., Gerhauser H. did CFD modeling [18] of fast pyrolysis of biomass in an Entrained Flow Reactor (EFR).The Lagrangian approach is adopted for the particle tracking, while the flow of the inert gas is treated with the standard Eulerian method for gases. The model includes the thermal degradation of biomass to char with simultaneous evolution of gases and tars from a discrete biomass particle. The chemical reactions are represented using a two-stage, semi-global model. The radial distribution of the pyrolysis products is predicted as well as their effect on the particle properties. The convective heat transfer to the surface of the particle is computed using the Ranz-Marshall correlation.

Baggio P., Baratieri M., Fiori L., Grigiante M., Avi D., Tosi P. [1]did Experimental and modeling analysis of a batch gasification/pyrolysis reactor.This paper presents some experimental results about biomass gasification obtained with a bench-scale gasifier consisting of an indirectly heated batch reactor, inserted in a high temperature furnace.The experimental activity includes the analysis of the thermal response of the system (using an inert bed material) and the characterization of the gasification products.The experimental results have been compared against calculations obtained by applying a thermochemical equilibrium model, improved to predict both the gas and the solid phase product yields.

Pallares Javier, Arauzo Inmaculada, [17] Williams Alan developed a new methodology using zone method and CFD codes.CFD solutions were obtained of the combustion conditions in the furnace in the Lamarmora power plant (ASM Brescia, Italy) for a number of different conditions and for three coals. Then, these furnace conditions were used as inputs for a more detailed chemical combustion model to predict coal burnout. In this, devolatilization was modelled using a commercial macromolecular network pyrolysis model (FG-DVC). For char oxidation an intrinsic reactivity approach including thermal annealing, ash inhibition and maceral effects, was used. Results from the simulations were compared against plant experimental values, showing a reasonable agreement in trends and quantitative values.

Habibi A., Merci B., Heynderickx G.J. [11] performed a three-dimensional (3-D) simulation of the flow in an industrial scale steam cracking furnace.The re-normalization group (RNG) $k-\epsilon$ turbulence model is used. The combustion kinetics is modeled by a three-step reaction mechanism, while turbulencechemistry interaction is taken into account through the Finite Rate/Eddy-Dissipation model. The Discrete Ordinates model (DOM), the P-1 and the Rosseland Radiation model are used for modeling of the radiative heat transfer. The results of using the different radiation models are compared mutually with adiabatic simulation results. The absorption coefficient of the gas mixture is calculated by means of a Weighted-Sum-of-Gray-Gas model (WSGGM). The effect is discussed of the use of different radiation models on the predicted wall, tube skin and flue gas temperature profiles and heat fluxes towards the reactor tubes, as well as on the predicted species concentration profiles and structure of the furnace flames under normal firing conditions.

Gerun Luc et al.[8] made 2D axisymmetric CFD model of the oxidation zone in a two-stage downdraft gasifier.The purpose of this study is to investigate in detail this zone, which is crucial for tar cracking. Results fit satisfactorily to the experimental data regarding temperature pattern and tar concentration.Simulations highlighted several crucial points of the process:(a)pyrolysis gas composition significantly influences the process (b)the air injector design is fundamental in gasification as the air velocity and the air/fuel ratio have a great influence on the process.

2.7 Aim and objectives of the study

The objectives of the thesis are listed below:

- The research objective of this study is to develop a 2-Dimensional Gasifier Model for Biomass Gasification using FLUENT 6.2.16. The overall aim is to study the validity of lignite gasifier.

- The numerical simulation model presented in this study is aimed at direct combustion in biomass gasifier. This gasifier offered a number of characteristics when such as intense burning, enhanced heat transfer, capability of improving pressure and in addition, some potential for improvements to effectiveness and efficiency especially in gas turbine for power production.

- Using the CFD (Computational Fluid Dynamics) commercial software, FLUENT 6.2.16, the study would continue to seek to understand the combustion mechanism of lignite in gasifier and then use this at larger scale to advantage for devices where fast accurate hot gas stream are needed in industrial and home appliances. In particular, to seek the fluid dynamics of the flow which is heavily dependent on the outlet channel characteristics.

- In the simulation part of the project, a model of down-draft gasifier consistent with main observed phenomena was proposed. To adapt the model for numerical analysis, a method was presented. In this method, as a preliminary approach,laminar and steady state combustion in the gasifier was simulated.

- Some results obtained from both numerical methods were compared with the experimental work carried out by Rohera Vinay (2009) and Dr. Patel R.N. On this basis, the validity of proposed model will be discussed.

Chapter 3

Basics of CFD

3.1 Introduction

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surfaces defined by boundary conditions. With high-speed supercomputers, better solutions can be achieved. Ongoing research, however, yield software that improves the accuracy and speed of complex simulation scenarios such as transonic or turbulent flows. Initial validation of such software is performed using a wind tunnel with the final validation coming in flight tests.

3.2 CFD Modeling Principles

Computational fluid dynamics is a design and analysis tool that uses computers to simulate fluid flow, heat and mass transfer, chemical reactions, solid and fluid interaction and other related phenomena. Comparing to the physical experiment operation, CFD modeling is cost saving, timely, safe and easy to scale-up. CFD codes turn computers into a virtual laboratory and perform the equivalent “numerical experiments conveniently providing insight, foresight and return on investment. Various numerical techniques known as direct numerical simulation (DNS), vortex dynamics and discretization methods have been employed in the solution of the CFD model equations. The most widely used numerical techniques are discretization methods mainly including finite difference (usually based on Taylors series, polynomial expansions), finite elements (based on calculus of variations, and the method-of-weighted-residuals) and finite volumes method (based on control volume formulation). Finite difference techniques are rarely used in engineering flows due to the difficulties in the handling of complex geometry [4]. Finite elements are used in the commercial packages of FIDAP and POLYFLOW. Finite volumes are now the most commonly used approach in CFD code development for its ease in the understanding, programming and versatility. The most routinely used commercial codes include ANSYS FLUENT, ANSYS CFX, PHOENICS, STAR-CD and CFD2000. The available commercial CFD programmes review and the CFD performing process introduction can be found in Xia and Sun [9], Norton et al.[16].

3.3 Discretization methods

The stability of the chosen discretization is generally established numerically rather than analytically as with simple linear problems. Special care must also be taken to ensure that the discretization handles discontinuous solutions gracefully. The Euler equations and Navier-Stokes equations both admit shocks, and contact surfaces. Some of the discretization methods being used are:

a. Finite Volume Method

   The finite volume method (FVM) is a common approach used in CFD codes. The governing equations are solved over discrete control volumes. Finite volume methods recast the governing partial differential equations (typically the Navier-Stokes equations) in a conservative form, and then discretize the new equation. This guarantees the conservation of fluxes through a particular control volume. Though the overall solution will be conservative in nature, there is no guarantee that it is the actual solution. The finite volume equation yields governing equations in the form,

$$\frac{\delta}{\delta t}\int\int\int QdV + \int\int FdA = 0 \tag{3.1}$$

Where, Q is the vector of conserved variables, F is the vector of fluxes, V is the volume of the control volume element, and is the surface area of the control volume element.

b. Finite Element Method

The finite element method (FEM) is used in structural analysis of solids, but is also applicable to fluids. However, the FEM formulation requires special care to ensure a conservative solution. The FEM formulation has been adapted for use with fluid dynamics governing equations. Although FEM must be carefully formulated to be conservative, it is much more stable than the finite volume approach. However, FEM can require more memory than FVM. In this method, a weighted residual equation is formed:

$$Ri = \int\int\int WiQdV^e \tag{3.2}$$

Where *Ri* is the equation residual at an element vertex i, Q is the conservation equation expressed on an element basis, Wi is the weight factor, and V^e is the volume of the element.

c. Finite Difference Method

The finite difference method (FDM) has historical importance and is simple to program. It is currently only used in few specialized codes. Modern finite difference codes make use of an embedded boundary for handling complex geometries, making these codes highly efficient and accurate. Other ways to handle geometries include use of overlapping grids, where the solution is interpolated across each grid.

$$\frac{\delta Q}{\delta t} + \frac{\delta F}{\delta x} + \frac{\delta G}{\delta y} + \frac{\delta H}{\delta z} = 0 \tag{3.3}$$

Where Q is the vector of conserved variables, and F, G, and H are the fluxes in the x, y, and z directions respectively.

d. Boundary Element Method

In the boundary element method, the boundary occupied by the fluid is divided into a surface mesh.

e. High Resolution Discretization Schemes

High-resolution schemes are used where shocks or discontinuities are present. Capturing sharp changes in the solution requires the use of second or higher-order numerical schemes that do not introduce spurious oscillations. This usually necessitates the application of flux limiters to ensure that the solution is total variation diminishing.

3.4 Theoretical considerations in CFD

The CFD codes are arranged by the numerical algorithm accordingly, so that the fluid flow problem can be tackled.There are three main elements of CFD codes in the CFD packages which consist of pre-processor, solver and post-processor.

3.4.1 Pre-processor

The pre-processor contains all the fluid flow inputs for a flow problem. It can be seen as a user-friendly interface and a conversion of all the input into the solver in CFD program. In this stage, quite a lot of activities are carried out before the problem is being solved. These stages are listed as below:

- Definition of the geometry

  The region of interests which is the computational domain.

- Grid generation

  The subdivision of the domain into a number of smaller and non overlapping domains. The grid mesh of cells is carried out for the geometry.

- Selection of the physical and chemical properties

  The geometry to be modeled.

- Definition of the fluid properties

- Specifications of correct boundary conditions

  This is done at model's cells. The solution of the flow problem such as temperature, velocity, pressure etc. is defined at the nodes insides each cell. The accuracy of the CFD solution governed by the number of cells in the grid and is dependent on the fineness of the grid.

3.4.2 Solver

In the numerical solution technique, there are three different streams that form the basis of the solver. There are finite differences, finite element and finite volume methods. The differences between them are the way in which the flow variables are approximated and the discretization processes are done.

- Finite difference element, FDM Describes the unknown flow variables of the flow problem by means of point samples at node points of a grid coordinate. By FDM, the Taylor's expansion is usually used to generate finite differences approximation.

- Finite element method, FEM Use the simple piecewise functions valid on elements to describe the local variations of unknown flow variables. Governing equation is precisely satisfied by the exact solution of flow variables. In FEM, residuals are used to measure the errors.

- Finite volume method, FVM It was originally developed as a special finite difference formulation. The main computational commercial CFD codes packages using the FVM approaches involves PHOENICS, FLUENT, FLOW 3D and STAR-CD. Basically, the numerical algorithm in these CFD commercial packages involved the formal integration of the governing equation over all the finite control volume, the discretization process involves the substitution of variety FDM types to approximate the integration equation of the flow problem and the solution is obtained by iterative method.

Discretization in the solver involves the approaches to solve the numerical integration of the flow problem. Usually, two different approaches have been used and once at a time.

- Explicit approach Usually, this is the most approach that makes sense. It is relatively simple to set up and program. The limitation is that for a given Δt and Δx, must be less than some limit imposed by stability constraints. In some cases, Δt must be very small to maintain the stability and consequently long running time required for the calculation over a given time interval, t.

- Implicit approach For this approach, the stability can be maintained over a large value of Δt and fewer time steps required making calculation. Thus resulting less computer time. Adversely, it is complicated to set up and program. The computer time per time step is much larger than the explicit approach due to the matrix manipulation which is required for each time step. This approach is very accurate to follow the exact transients i.e. the time variations of the independent variables.

3.4.3 Post-processor

A FLUENT package provides the data visualization tools to visualize the flow problem. This includes - vectors plots, domain geometry and grid display, line and shaded counter plots, particle tracking etc. Recent facilities aided with animation for dynamic result display and also have data export facilities for further manipulation external to the code.

3.5 Problem solving

In the computational fluid dynamics, using the FLUENT codes provide to solve the problem numerically. The fundamental involves determining the convergence, whether the solution is consistent and stable for all range of flow variables.

- Convergence - is a property of a numerical method to produce a solution that approaches the exact solution of which the grid spacing, control volume size is reduced to a specific value or to zero value.
- Consistent - to produce the system of algebraic equations, which can be equivalent to the original governing equation.
- Stability - associates with the damping of errors as a numerical method proceeds. If a technique chosen is not stable, even the round-off error in the initial data can leads to wild oscillations or divergence.

3.6 Solution Methodology

The pre-processing tool used in this study is GAMBIT, which provides one interface to build and mesh the geometry. The CFD solver is the commercial CFD code FLUENT Version 6.1.22. FLUENT is a finite-volume-based CFD solver written in C language, and has the ability to solve fluid flow, heat transfer and chemical reactions in complex geometries and supports both structured and unstructured mesh.The geometry is generated and meshed in GAMBIT. Two-dimensional Triangular mesh is used for meshing the gasifier. A total of 54,430 cells are employed. After the model has been meshed, it is exported to FLUENT.

3.6.1 Numerical Procedure

The procedure for performing the simulation in FLUENT is outlined below.

a. Create and mesh the geometry model using GAMBIT

b. Import geometry into FLUENT

c. Define the solver model

d. Define the turbulence model

e. Define the species model

f. Define the radiation model

g. Define the materials and the chemical reactions

h. Define the boundary conditions

i. Initialize the calculations

j. Iterate/calculate until convergence is achieved

k. Post-process the results

FLUENT offers two solution methods: (a) segregated solution and (b) coupled solution. Segregated solution solves the governing equations of continuity, momentum, energy, and species transport sequentially (segregated from one another). On the other hand, coupled solution solves the governing equations of continuity, momentum, energy, and species transport simultaneously. The equations for scalars such as turbulence and radiation are solved using the previously updated values from the momentum equations. Segregated solution is chosen for this study. The detailed steps of segregated solution are given below.

a. Fluid properties are updated based on the current solution or the initialized solution.

b. The momentum equations are solved using the current values of pressure and face mass fluxes to get the updated velocity field.

c. Equation for the pressure correction is calculated from the continuity equation and the linearized momentum equations since the velocity field obtained in step (ii) may not satisfy the continuity equation.

d. The pressure correction equations obtained from step (iii) are solved to correct the pressure and velocity fields, and face mass such that the continuity equation is satisfied.

e. The equations for scalars such as turbulence, energy, radiation, and species are solved using the updated values of the other variables.

f. The equation is checked for convergence.

These steps are repeated until the convergence criteria are met.

The non-linear governing equations can be linearized implicitly or explicitly with respect to the dependent variables. If linearized implicitly, the unknown value in each cell is computed using a relation that includes both existing and unknown values from neighboring cells. If linearized explicitly, the unknown value in each cell is computed using a relation that includes only existing values. In the segregated solution, the linearization is implicit. Therefore, each unknown will appear in more than one equation in the linear system, and these equations must be solved simultaneously to give the unknown quantities.

FLUENT uses a control-volume-based technique to convert the governing equations to algebraic equations, which are then solved mathematically. The discretization of the governing equations yields discrete equations that conserve each quantity on a control-volume basis. There are several discretization schemes available in FLUENT: (a) First Order, (b) Second Order, (c) Power Law, and (d) QUICK. The first order discretization scheme is applied for the momentum, the turbulence kinetic energy, the turbulence kinetic dissipation, the energy, and all the species.

FLUENT provides three algorithms for pressure-velocity coupling in the segregated solver: (a) SIMPLE, (b) SIMPLEC, and (c) PISO. The SIMPLE algorithm [20] is used in this study. The built-in standard $k - \epsilon$ turbulence model is used. FLUENT offers several species model: Species transport: laminar finite-rate, eddy-dissipation, or eddy-dissipation concept (EDC).

- Non-premixed combustion
- Premixed combustion
- Partially premixed combustion
- Composition PDF combustion

The species model and transport model with volumetric reaction are chosen to simulate the diffusion and production/destruction of the chemical species. The eddy dissipation model is utilized to calculate the net production and destruction of the species. Eddy-dissipation model assumes that chemical kinetics is fast compared to the mixing rate of the reactants by the turbulent fluctuations.A mixture material that consists of seven chemical species (C, O_2, N_2, CO, CO_2, H_2O and H_2) is defined. All the species, including C, are defined as fluid species and are assumed to mix at the molecular level. The specific heat of the species is temperature dependant and is defined as a piecewise-polynomial function of temperature.

Before FLUENT can begin solving governing equations, flow field guessed initial values, used as the initial values of the solution, have to be provided. Once the initial values have been provided, the iteration is performed until a converged result is obtained.

Chapter 4

Modeling and Simulation

Computational fluid dynamics is a design and analysis tool that uses computers to simulate fluid flow, heat and mass transfer, chemical reactions, solid and fluid interaction and other related phenomena. Comparing to the physical experiment operation, CFD modeling is cost saving, timely, safe and easy to scale-up.For the gasifier systems,the chemistry of the gasification equations are modeled.Homogeneous as well as heterogeneous reactions are modeled in the Fluent and finally they are simulated for the number of iterations.

4.1 Gasification Equation

In a gasifier, various chemical reactions take place inside the system. These reactions can be broadly divided into 2 categories i.e. homogenous reaction and non-homogenous (heterogeneous) reactions:

- **Heterogeneous reactions** These reactions involve multiple phases. In a gasifier, many solid-gas reactions occur in the gasification zone that comes under this category. Some of these reactions include:
  Reaction 1: Boudouard reaction:

$$C + CO_2 \leftrightarrow 2CO \tag{4.1}$$

Reaction 2: Water gas (primary) reaction:

$$C + H_2O \leftrightarrow CO + H_2 \tag{4.2}$$

Reaction 3: Methanation reaction:

$$C + 2H_2 \leftrightarrow CH_4 \tag{4.3}$$

Reaction 4: Steam reforming reaction:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \tag{4.4}$$

Reaction 5: Water gas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \tag{4.5}$$

- **Homogenous reactions** The homogenous reactions occur in a single phase and mainly constitute of gas phase reactions including:

$$2H_2 + O_2 \rightarrow H_2O \tag{4.6}$$

$$CO_2 + H_2 \rightarrow CO + H_2O \tag{4.7}$$

4.2 Model Formulation

The geometry of the gasifier used in the simulation is shown in Fig 4.1The gasifier is divided into four regions: a combustion region near the throat, a reduction region above the combustion zone, oxidation zone above the reduction zone and finally drying zone above oxidation region. lower stage. The gasifier has three levels of air tuyeres that are positioned at the top of the gasifier.All the three tuyeres are aimed at the throat inside the gasifier.Lignite is already filled in the gasifier.

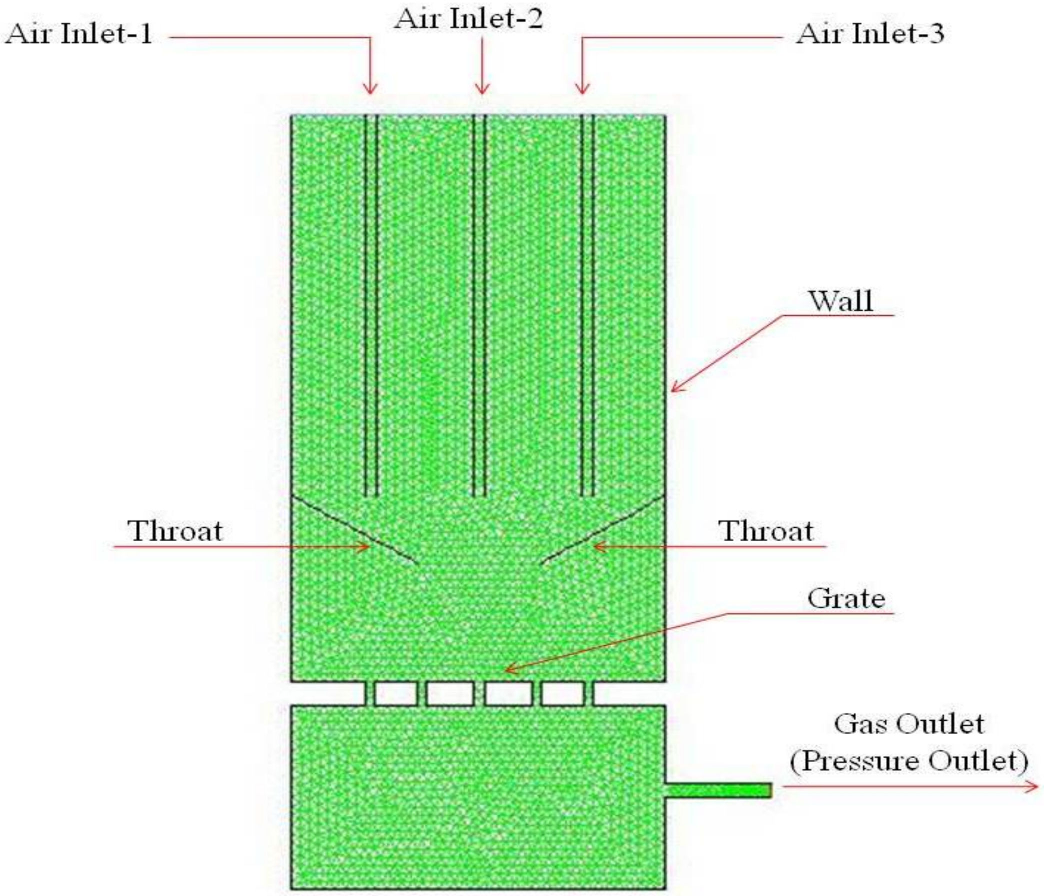

Figure 4.1: Grid

4.2.1 Physical Characteristics of the Problem and Assumptions Made

Nevertheless, the present computational fluid dynamic models are unable to solve such complex reaction mechanisms due to its complexity. Employing detailed reaction mechanisms in the CFD calculations will generate a numerically inflexible problem that it will be difficult to reach converged solution with the present of the solver in the CFD commercial software.

Brink et al [5] created a model for biomass combustion using single-step mechanics and turbulence-chemistry interaction with eddy dissipation combustion model as the air distribution were injected around the bottom of the model. Therefore, the use of much simple or single-step reaction mechanisms is preferred rather than the global reaction mechanism.

The physical characteristics of the problem are as follow:

a. 2 - Dimensional

b. Bouyancy force considered

c. Varying fluid properties

d. Impermeable walls

The following are the general assumptions made in this study:

- Low Mach number for the combustion approximation
- Single-phase gaseous flow of ideal gas
- Neglect the electromagnetic radiation
- Simplified chemistry i.e. single step, Arrhenius
- Newtonian fluid flow; Fouriers and Ficks law for the diffusion heat and mass transfer

The assumption of the low Mach number implies that the ambient flow speeds are low that the heat release rate is not so strong i.e. no blast waves. The density variations are due to the differences of the density of the reaction species and the chemically reaction heat release rate.

4.2.2 Governing Equations

The equations for conservation of mass, conservation of momentum, and energy equation are given as:

$$\nabla \cdot (\rho \overrightarrow{\nu}) = S_m \tag{4.8}$$

$$\nabla \cdot (\rho \overrightarrow{\nu} \overrightarrow{\nu}) = -\nabla p + \nabla \cdot (\overline{\tau}) + \rho \overrightarrow{g} + \overrightarrow{F} \tag{4.9}$$

$$\nabla \cdot (\nu(\rho E + p)) = \nabla \cdot (\lambda_{eff} \nabla T - \sum h_j J_j + (\overrightarrow{\tau}_{eff} \cdot \overrightarrow{\nu})) + S_h \tag{4.10}$$

Where, λ_{eff} is the effective conductivity (l+lt, where lt is the turbulence conductivity) and J_j is the diffusion of species j.

The stress tensor is given by,

$$\overline{\tau} = \mu[(\nabla \overrightarrow{\nu} + \nabla \overrightarrow{\nu}^T) - \frac{2}{3} \nabla \cdot \overrightarrow{\nu} I] \tag{4.11}$$

where m is the molecular dynamic viscosity, I is the unit tensor, and the second term on the right-hand side is the effect of volume dilatation. The first three terms on the right hand side of equation represent heat transfer due to conduction, species diffusion, and viscous dissipation. $S_h$is a source term including the enthalpy formation from the chemical reaction of the species.

4.2.3 Turbulence Model

The velocity field in turbulent flows always fluctuates. As a result, the transported quantities such as momentum, energy, and species concentration fluctuate as well.

The fluctuations can be small scale and high frequency, which is computationally expensive to be directly simulated.So the modifications are being made. However, the modifications of the instantaneous governing equations introduce new unknown variables.[14] Many turbulence models have been developed to determine these new unknown variables in terms of known variables. General turbulence models widely available are:

a. Spalart-Allmaras

b. $k - \epsilon$ models

  - Standard k-ϵ model
  - RNG k-ϵ model
  - Realizable k-ϵ model

c. k-w models

  - Standard k-w model
  - Shear-stress transport (SST) k-w model

d. Reynolds Stress

e. Large Eddy Dissipation

The standard k-ϵ turbulence model, which is the simplest two-equation turbulence model, is used in this simulation due to its suitability for a wide range of wall-bound and free shear flows. The standard k-ϵ turbulence is based on the model transport equations for the turbulence kinetic energy, k, and its dissipation rate, ϵ. The model transport equation for k is derived from the exact equation; however, the model transport equation for ϵ is obtained using physical reasoning.The standard k-ϵ turbulence model is robust, economic for computation, and accurate for a wide range of turbulent flows. The turbulence kinetic energy, k, and its rate of dissipations, ϵ , are calculated from the following equations

$$\frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}[(\mu + \frac{\mu}{\sigma_k})\frac{\partial k}{\partial x_j}] + G_k + G_b - \rho\epsilon - Y_M + S_k \tag{4.12}$$

and

$$\frac{\partial}{\partial x_i}(\rho\epsilon u_i) = \frac{\partial}{\partial x_j}[(\mu + \frac{\mu}{\sigma_\epsilon})\frac{\partial \epsilon}{\partial x_j}] + C_{1\epsilon}\frac{\epsilon}{k}(G_k + C_{3\epsilon}G_b) - C_{2\epsilon}\rho\frac{\epsilon^2}{k} + S_\epsilon \tag{4.13}$$

In the equations 4.12 and 4.13 G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients and is defined as

$$G_k = -\overline{\rho u_i' u_j'}\frac{\partial u_j}{\partial x_j} \tag{4.14}$$

G_b represents the generation of turbulence kinetic energy due to buoyancy and is calculated as

$$G_b = \beta g_i \frac{\mu_t}{Pr_t}\frac{\partial T}{\partial x_i} \tag{4.15}$$

P_{rt} is the turbulent Prandtl number and gi is the component of the gravitational vector in the i^{th} direction. For standard k-ϵ model the value for P_{rt} is set 0.85.

Y_M represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, and is defined as

$$Y_M = 2\rho\epsilon M_t^2 \tag{4.16}$$

where, M_t is the turbulent Mach number which is defined as

$$M = \sqrt{\frac{k}{a^2}} \tag{4.17}$$

where, a ($\sqrt{\gamma RT}$) is the speed of sound.
The values of constants $C_{1\epsilon}$, $C_{2\epsilon}$, C_m, S_k and S_e used are $C_{1\epsilon}$ = 1.44, $C_{2\epsilon}$ = 1.92,C_m = 0.09,S_k = 1.0, S_e= 1.3.

The solution in the near-wall region can be very important because the solution variables have large gradients in this region. [14] However, the solution in the boundary layer is not important in this study.Wall functions, which are the collection of semi-empirical formulas and functions, are employed to connect the viscosity-affected region between the wall and the fully-turbulent region.

4.2.4 Combustion Model

The global reaction mechanism is modeled to involve the following chemical species:C, O_2, CO, CO_2, H_2O and H_2.All of the species are assumed to mix in the molecular level. The chemical reactions inside the gasifier are modeled by calculating the transport and mixing of the chemical species by solving the conservation equations describing convection, diffusion, and reaction of each component species.
The transport equations for each chemical species are:

$$\frac{\partial}{\partial t}(\rho Y_C) + \nabla(\rho \overline{v} Y_C) = -\nabla \overline{J}_C + R_C \tag{4.18}$$

$$\frac{\partial}{\partial t}(\rho Y_{O_2}) + \nabla(\rho \overline{v} Y_{O_2}) = -\nabla \overline{J}_{O_2} + R_{O_2} \tag{4.19}$$

$$\frac{\partial}{\partial t}(\rho Y_{N_2}) + \nabla(\rho \overline{v} Y_{N_2}) = -\nabla \overline{J}_{N_2} + R_{N_2} \tag{4.20}$$

$$\frac{\partial}{\partial t}(\rho Y_{CO}) + \nabla(\rho\overline{\nu}Y_{CO}) = -\nabla\overline{J}_{CO} + R_{CO} \tag{4.21}$$

$$\frac{\partial}{\partial t}(\rho Y_{CO_2}) + \nabla(\rho\overline{\nu}Y_{CO_2}) = -\nabla\overline{J}_{CO_2} + R_{CO_2} \tag{4.22}$$

$$\frac{\partial}{\partial t}(\rho Y_{H_2}) + \nabla(\rho\overline{\nu}Y_{H_2}) = -\nabla\overline{J}_{H_2} + R_{H_2} \tag{4.23}$$

$$\frac{\partial}{\partial t}(\rho Y_{H_2O}) + \nabla(\rho\overline{\nu}Y_{H_2O}) = -\nabla\overline{J}_{H_2O} + R_{H_2O} \tag{4.24}$$

The reaction equations that need to be solved are given below:

$$C + CO_2 = 2CO_2 \tag{4.25}$$

$$C + H_2O = CO + H_2 \tag{4.26}$$

$$C + H_2 = CO + H_2O \tag{4.27}$$

$$C + 2H_2 = CH_4 \tag{4.28}$$

$$C + 3H_2 = CH_4 + H_2O \tag{4.29}$$

There are three approaches to solving these reactions:

- Eddy-dissipation model: The assumption in this model is that the chemical reaction is faster than the time scale of the turbulence eddies. Thus, the reaction rate is determined by the turbulence mixing of the species. The reaction is assumed to occur instantaneously when the reactants meet.

- Equilibrium model: The rate of chemical reaction is governed by the rate of mixing of gaseous oxidant and reactant. The reactions are fast compare to the time scale of turbulence. The gaseous properties become functions of the turbulent mixing rate and can be calculated using equilibrium considerations.
- Reaction rate model: The rate of chemical reaction is computed using an expression that takes into account temperature and pressure and ignores the effects of the turbulent eddies.

In the present study, the eddy-dissipation model is used.

4.2.5 Radiation Model

The radiative transfer equation (RTE) for an absorbing, emitting, and scattering medium at position $\overrightarrow{r}$ in the direction $\overrightarrow{s}$ can be written as follows:

$$\frac{dI(\overrightarrow{r}, \overrightarrow{s})}{dS} + (a + \sigma_s) I(\overrightarrow{r}, \overrightarrow{s}) = an^2 \frac{\sigma T^4}{\Pi} + \frac{\sigma_s}{4\Pi} \int I(\overrightarrow{r}, \overrightarrow{s}') \quad \Phi(\overrightarrow{r}, \overrightarrow{s}') d\Omega' \quad (4.30)$$

A semi-transparent medium is considered and the refractive index is equal to unity. The optical thickness aL where L is an appropriate length scale is a good indicator of which model to use. When $aL >> l$ the P-1 and Rosseland models are suitable.The P-1 model should typically be used for optical thicknesses large than 1. The Rosseland model is computationally cheaper and more efficient but should only be used for optical thicknesses larger than 3.

- P-1 Model

  P-1 model is the simplest formulation of the more general P-N radiation model, which is based on the expansion of the radiation intensity I into an orthogonal series of spherical harmonics. The method of spherical harmonics provides a vehicle to obtain an approximate solution of arbitrary high order (i.e. accuracy), by transforming the radiative transfer equation into a set of simultaneous partial differential equations.Using only four terms in the series solution of the respective differential equation, the following relation is obtained for the radiation flux:

$$q_r = \frac{1}{3(\alpha + \sigma_s) - C\Sigma_s} \nabla G \tag{4.31}$$

where G is the incident radiation. The problem is then much simplified since it is only necessary to find a solution for G rather than determining the direction dependent intensity.

- Rosseland model

  The Rosseland radiation model can be derived from the P-1 radiation model with some approximations. The radiative heat flux vector in a gray medium is approximated by

  $$\overrightarrow{q_r} = -\Gamma \nabla G \tag{4.32}$$

  The Rosseland radiation model differs from the P-1 model in that the Rosseland model assumes the intensity equal to the black-body intensity at the gas temperature.This model is also called diffusion approximation model, since the radiation problem reduces to a simple conduction problem with strongly temperature dependent conductivity.

4.2.6 Mixture Fraction Model

The mixture fraction model is used to present the reaction chemistry in the probability density function (PDF) method for solving turbulent-chemistry interaction. The equilibrium model is applied which assumes that the chemistry is rapid enough for chemical equilibrium to always exist at the molecular level. Basing on the simplifying assumptions, the instantaneous thermo-chemical state of the fluid is related to the mixture fraction f . An algorithm based on the minimization of Gibbs free energy is used to compute species mole fractions from f . The mixture fraction f is defined in terms of the atomic mass fraction as:

$$f = \frac{Z_j - Z_{j,ox}}{Z_{j,fuel} - Z_{j,ox}} \tag{4.33}$$

where Z_j is the mass fraction for element j . The subscript *ox* and *fuel* denote the value at the oxidizer stream inlet and the fuel stream inlet respectively.

4.3 Boundary Conditions and Initial Conditions

The boundary condition for each segments in the gasifier are specified in FLUENT. FLUENT has a wide range of boundary conditions that permit flow to enter and exit the solution domain. FLUENT provides 10 types of boundary cell types for the specification of flow inlets and exits: velocity inlet, pressure inlet, mass flow inlet, pressure outlet, pressure far-field, outflow, inlet vent, intake fan, outlet vent, and exhaust fan. The inlet and exit boundary condition options in FLUENT that were used in this 2-dimensional model are as follows:

Velocity inlet boundary conditions are used to define the velocity and scalar properties of the flow at inlet boundaries.

Pressure inlet boundary conditions are used to define the total pressure and other scalar quantities at flow inlets.

Mass flow inlet boundary conditions are used in compressible flows to prescribe a mass flow rate at an inlet. It is not necessary to use mass flow inlets in incompressible flows because when density is constant, velocity inlet boundary conditions will fix the mass flow.

Pressure outlet boundary conditions are used to define the static pressure at flow outlets (and also other scalar variables, in case of back-flow). The use of a pressure outlet boundary condition instead of an outflow condition often results in a better rate of convergence when back-flow occurs during iteration.

Walls The outside surfaces are defined as wall boundary. The walls are stationary with no-slip condition imposed (zero velocity) on the surface. For adiabatic case, the heat flux on the wall is set to 0 (zero). For constant wall temperature, the wall temperature is set to a certain constant value.

4.4 Model Parameters Setting in FLUENT

- **Model --→ Settings**
- Space --→ 2-D
- Time --→ Steady
- Viscous --→ Std $k - \epsilon$
- Heat Transfer--→ Enabled
- Melting-Freezing --→ Disabled
- Radiation --→ P-1
- Species Transport --→ Non-premixed
- Coupled Disperse Phase --→ Disabled
- Pollutants --→ Disabled
- Soot --→ Disabled

4.4.1 Relaxation Factors

- **Variable--→Relaxation Factor**
- Pressure --→ 0.1

- Momentum --→ 0.1
- Energy --→ 0.899998
- Density --→ 1
- Body Forces --→ 1

4.4.2 Discretization Scheme

- **Variable --→ Scheme**
- Pressure --→ Standard
- Momentum --→ Second Order Upwind
- Energy --→ Second Order Upwind
- Pressure-Velocity Coupling --→ PISO
- *Ligvol* --→ Second Order Upwind

4.4.3 Material : Lignite Volatiles

- Calorific Value --→ 9300 $\frac{KJ}{Kg}$
- Density --→ 700 $\frac{Kg}{m^3}$
- Specific heat (C_p) --→ 4500 $\frac{j}{Kg-K}$
- Thermal Conductivity --→ 0.174 $\frac{W}{m-K}$

Proximate Analysis of coal

- Moisture % --→ 50
- Ash % --→ 10.41

- Volatile Matter % --→ 47.76
- Fixed carbon % --→ 41.83

Ultimate Analysis of coal

- C --→ 0.581
- H --→ 0.390
- O --→ 0.013
- N --→ 0.016
- S --→ 0

Chapter 5

Results and Discussion

The temperature and pressure history of a particle in the down-draft gasifier was the primary focus of a detailed characterization study as this relationship in theory could exclusively determine the extent to which the solid material reacts.Particle temperature is influenced by radiative and convective transport, internal conduction, chemical reaction and also most of it by hot wall impact.
A simple model is not sufficient to capture the complexity of these problems. CFD simulations were employed to model many of these complex processes as the geometry and input condition can be accurately measured. This is because the model boundary conditions are based on measured quantities.

5.1 Temperature Contours

According to the results from the simulation, the total temperature is mostly high around the throat and nozzle. The temperature is higher at these areas because it is affected by the flame/torch that is placed at the wall near the throat. Furthermore, these areas are oxidation zone and reduction zone where all the lignite is burnt.

The temperature decreases as the height of the gasifier increases.As adiabatic conditions are applied for the wall the temperature of the wall remains constant and heat is not dissipated outside the gasifier.Mostly the temperature at upstream

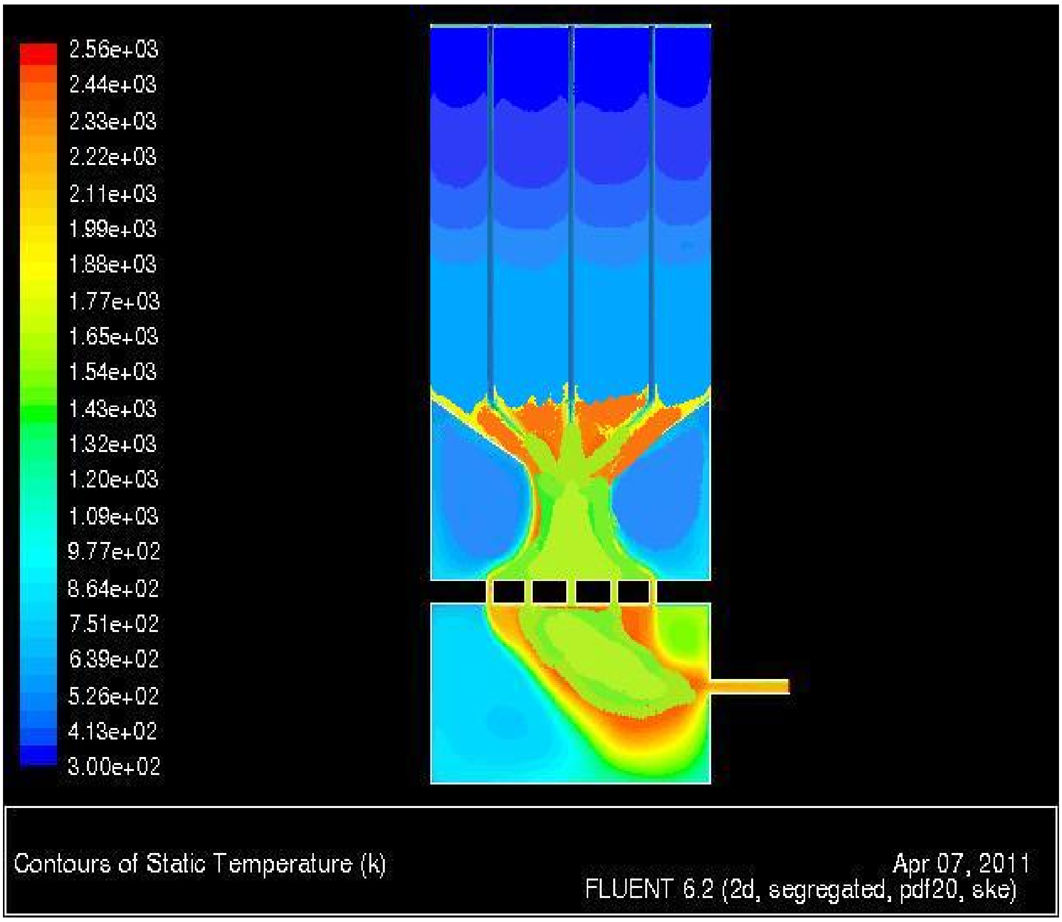

Figure 5.1: Temperature profile

and downstream of the gasifier remains around 310-350 K.The temperature of the combustion zone is 1378 K.The temperature of the reduction zone is in the range of 746-779 K.And finally,the temperature of the drying zone,which is above the pyrolysis zone, is 335 K.temperature of the reduction zone is quite high as 1743 K,which is practically not possible.

5.2 Filled velocity Profile

The velocity in the model lies between the range of 0.0360 m/s to 1.20 m/s.The highest velocity is achieved near the exhaust nozzle, which is at the downstream of the gasifier.

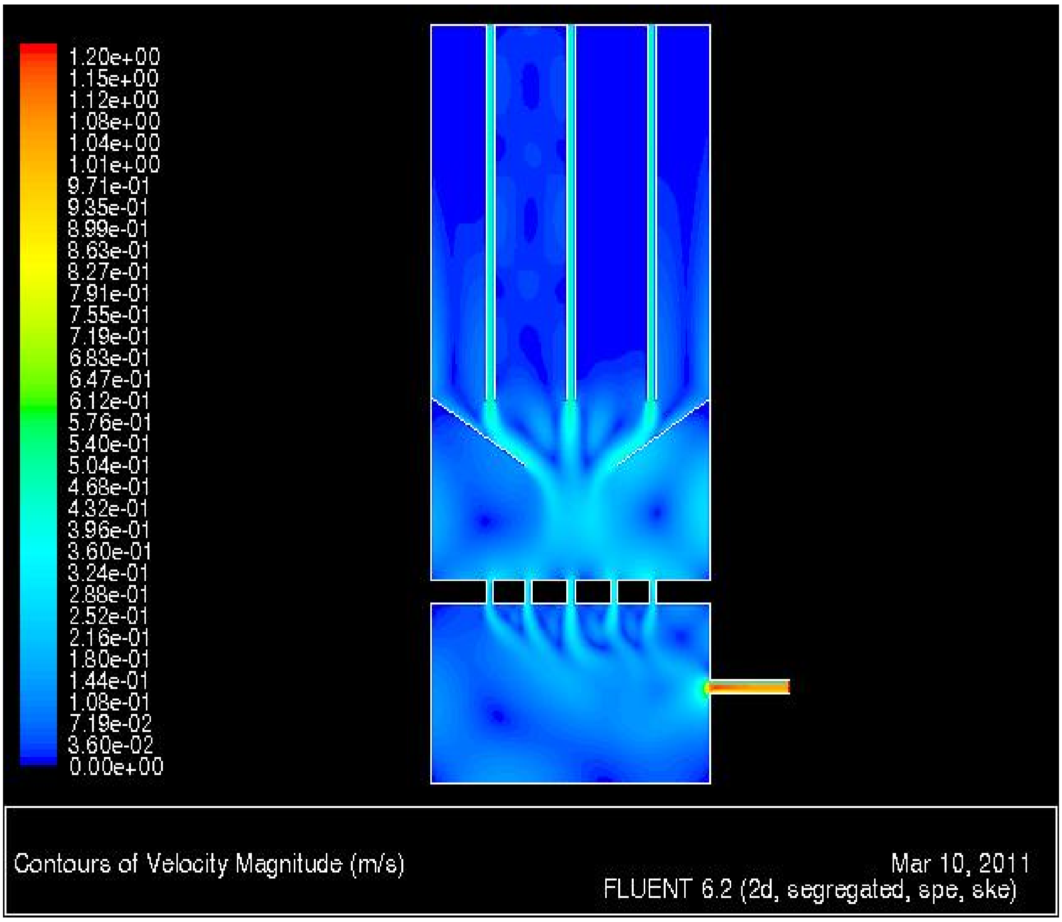

Figure 5.2: Velocity profile

The velocity contours 5.2slightly changes near the grate region as well as near the throat region. Whirling phenomenon is achieved when combustion of air is done but when the combustion of coal takes place this phenomenon is vanished.The above value of average velocity is taken when the combustion of coal and air is done.

5.3 Contours of Static Pressure

The temperature and pressure history of a particle in the down-draft gasifier was the primary focus of a detailed characterization study as this relationship in theory could exclusively determine the extent to which the solid material reacts. Particle temperature is influenced by radiative and convective transport, internal conduction, chemical reaction and also most of it by hot wall impact.

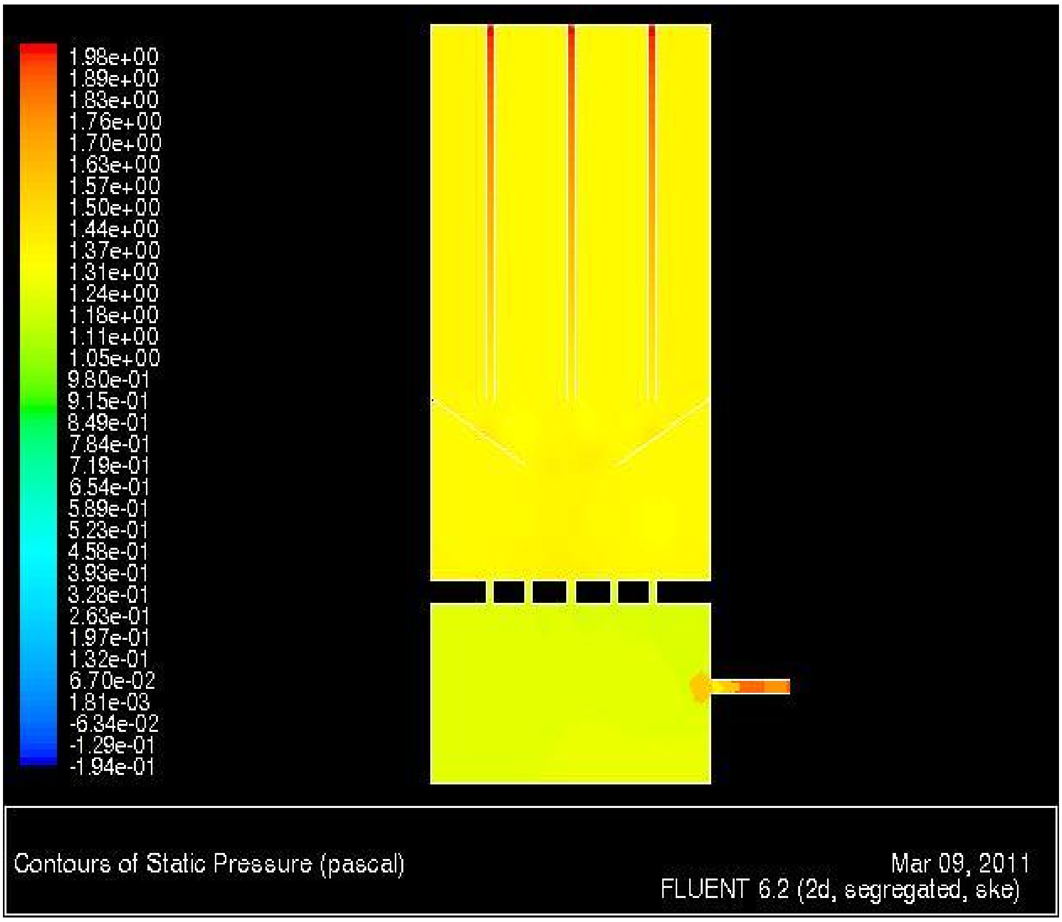

Figure 5.3: Static pressure profile

From the contour of static pressure5.3, there is not much different from predicted total pressure. The pressure distributions are roughly the same.The maximum static pressure is 1.98 pascal and minimum pressure is 1.11 pascal.There is only a minor change near the grate region and gas outlet nozzle region.

5.4 Mass Fraction of Lignite

It is seen from the figure that the particles of lignite are consumed in the combustion process.As the lignite is progressed in downward direction, the mass of lignite is changing.Below the throat region the coal particles are not seen because of the irregular distribution of coal particles.This results did not match with the practical solutions.

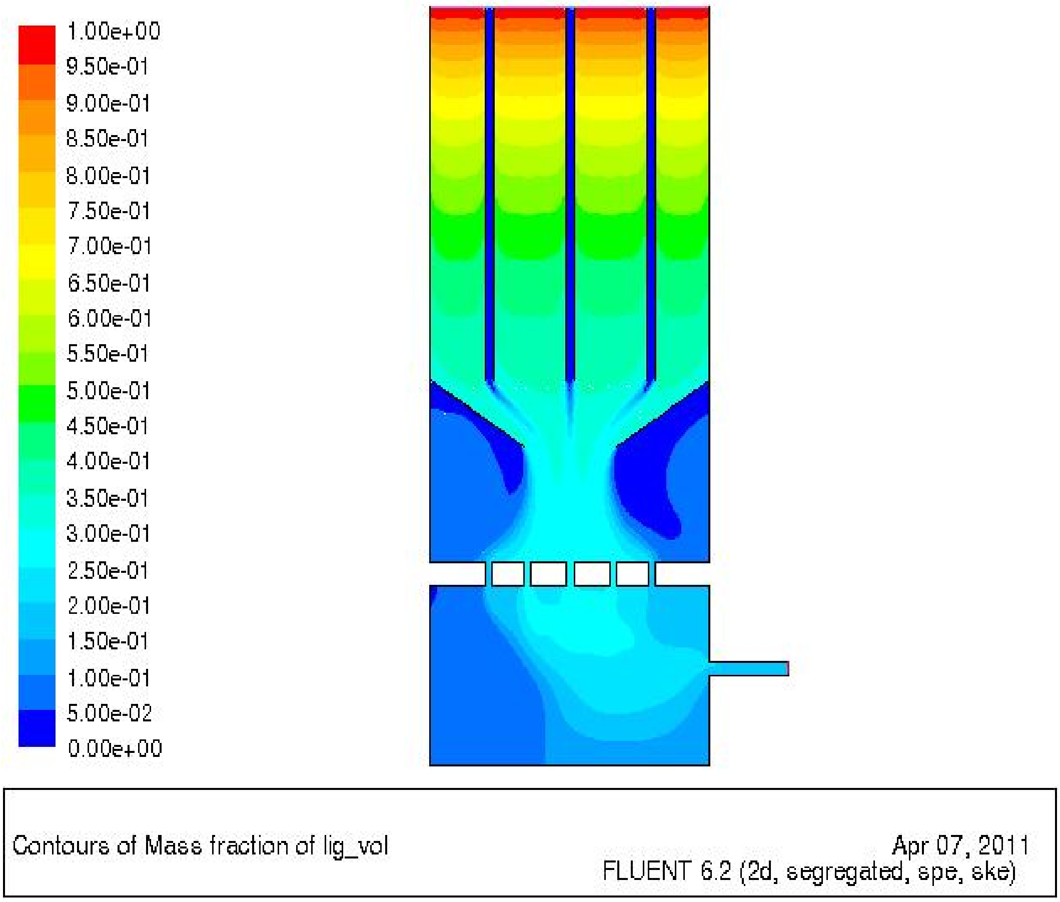

Figure 5.4: Mass fraction of lignite

5.5 Mass Fraction of C$< s >$

Having the correct gasification kinetics for char is critical for any gasifier model. It is clear from the figure5.5 that as the combustion of coal takes place the char and tar is been made from the coal.But near the throat region,the char-burnout factor is vanished i.e. char is no longer visible in the same region.

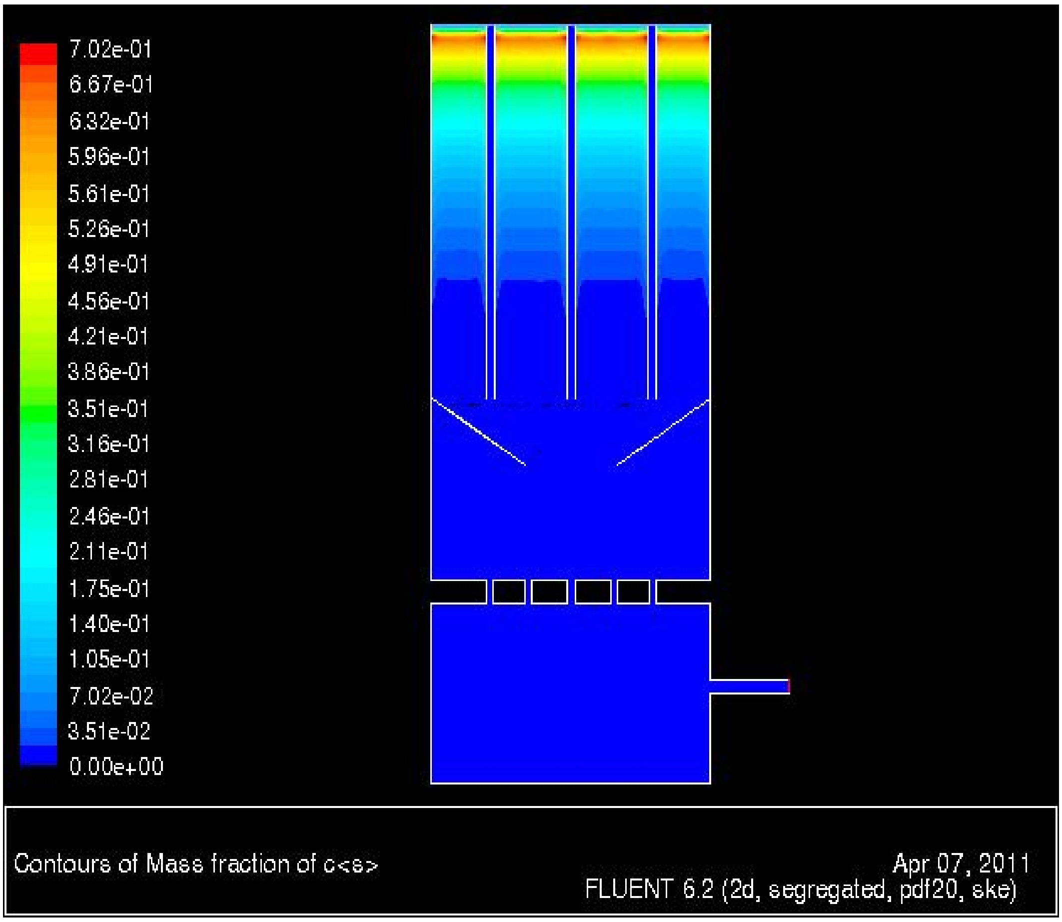

Figure 5.5: Mass fraction of char

5.6 Mass Fraction of CO

The results are matched with the practical solutions.5.6It is found that the mass fraction of CO is well enough in the pyrolysis zone.The amount of CO is decreased at the gas outlet nozzle which is practically not true.Althogh boundary conditions for the exhaust nozzle are changed,the results are not varying.There is not much difference between the results when the conditions are changed from pressure outlet to exhaust fan.

The amount of CO should vary between 10-30 %.And after the simulation ,the average amount of CO is found out to be 20 % which is quite convincing.

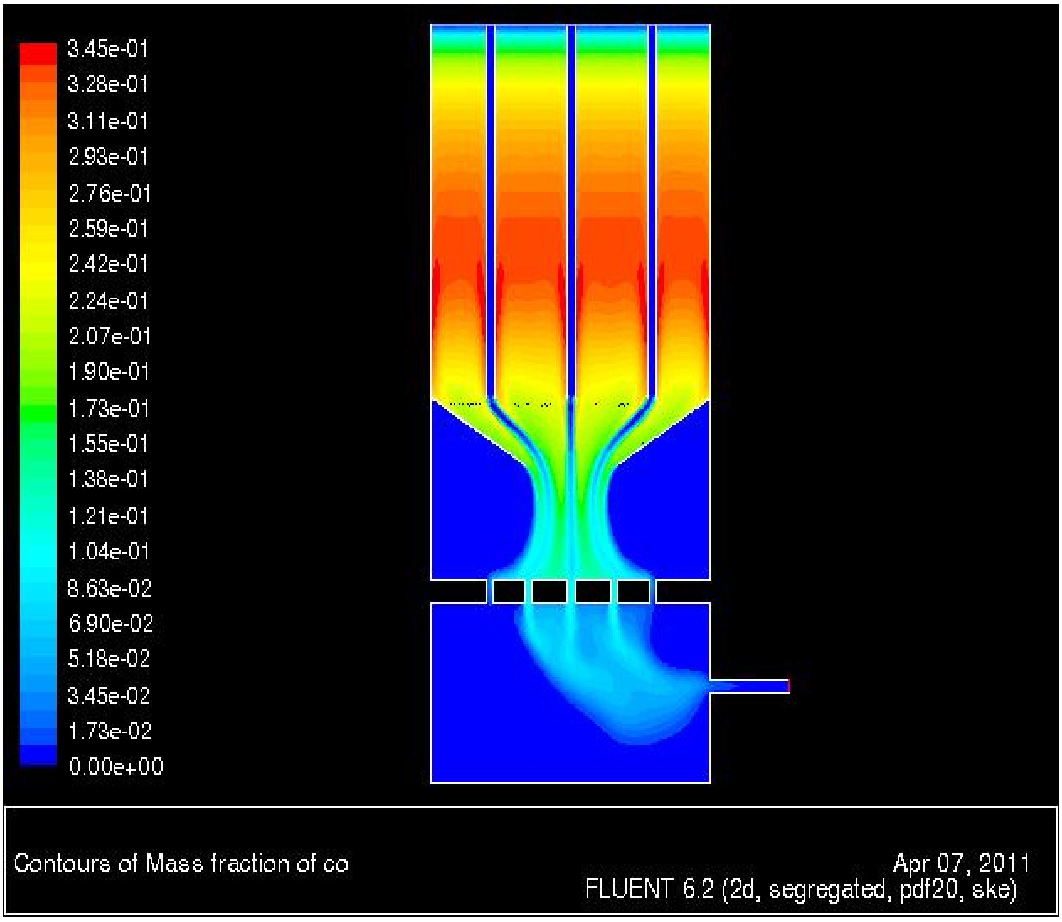

Figure 5.6: Mass fraction of CO

5.7 Mass Fraction of CO_2

From the fig 5.6 it is seen that the whole CO is remained only above the grate.The maximum mass fraction of CO_2 is found out to be 23.4 %.The reactive O molecules are found out maximum below the grate.

The concentration of CO_2 is highest at the exit of the chamber as the gas is going in outward direction.

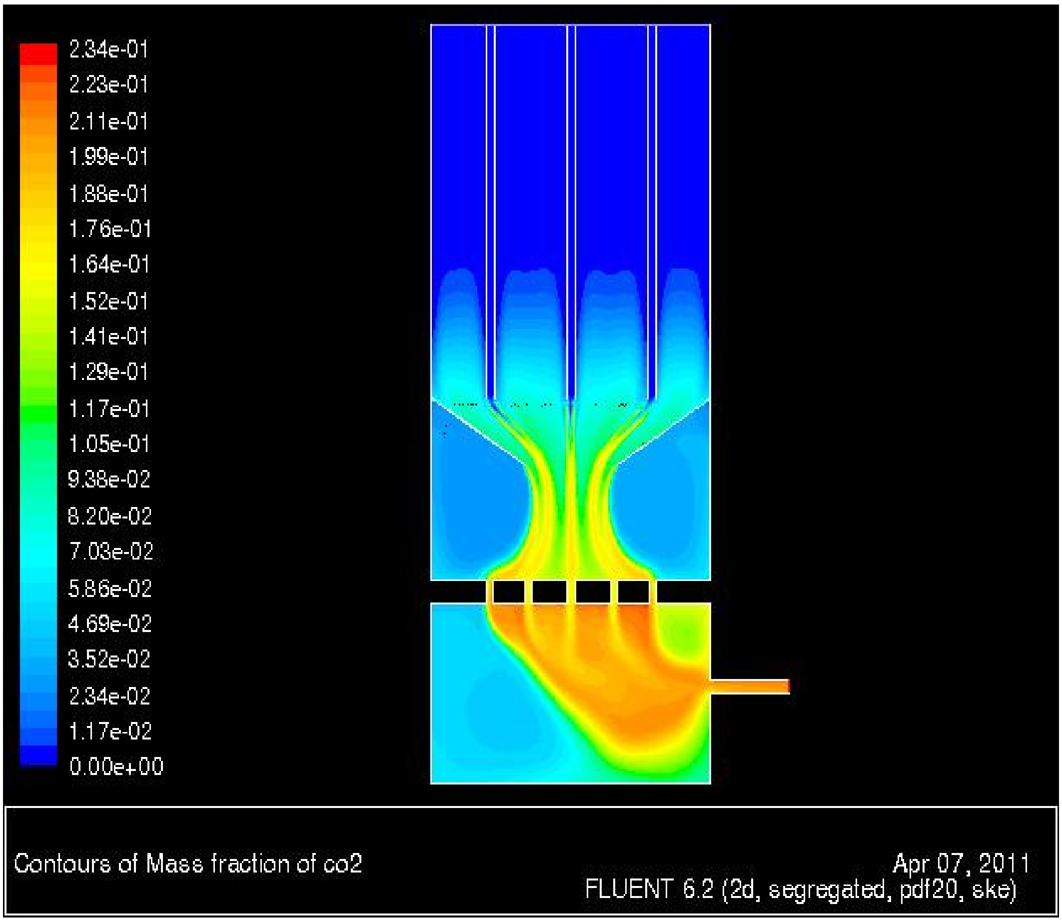

Figure 5.7: Mass fraction of CO_2

5.8 Mass Fraction of H_2O

The water-Gas shift reaction is in equilibrium throughout most of the reaction chamber.

There is some percentage of moisture in the lignite.But as and when the combustion initiates this moisture is vanished simultaneously.In the drying zone, minor portion of the H_2O is observed.But as the combustion is progressed,this H_2O is divided in to H_2 and O_2 molecules.

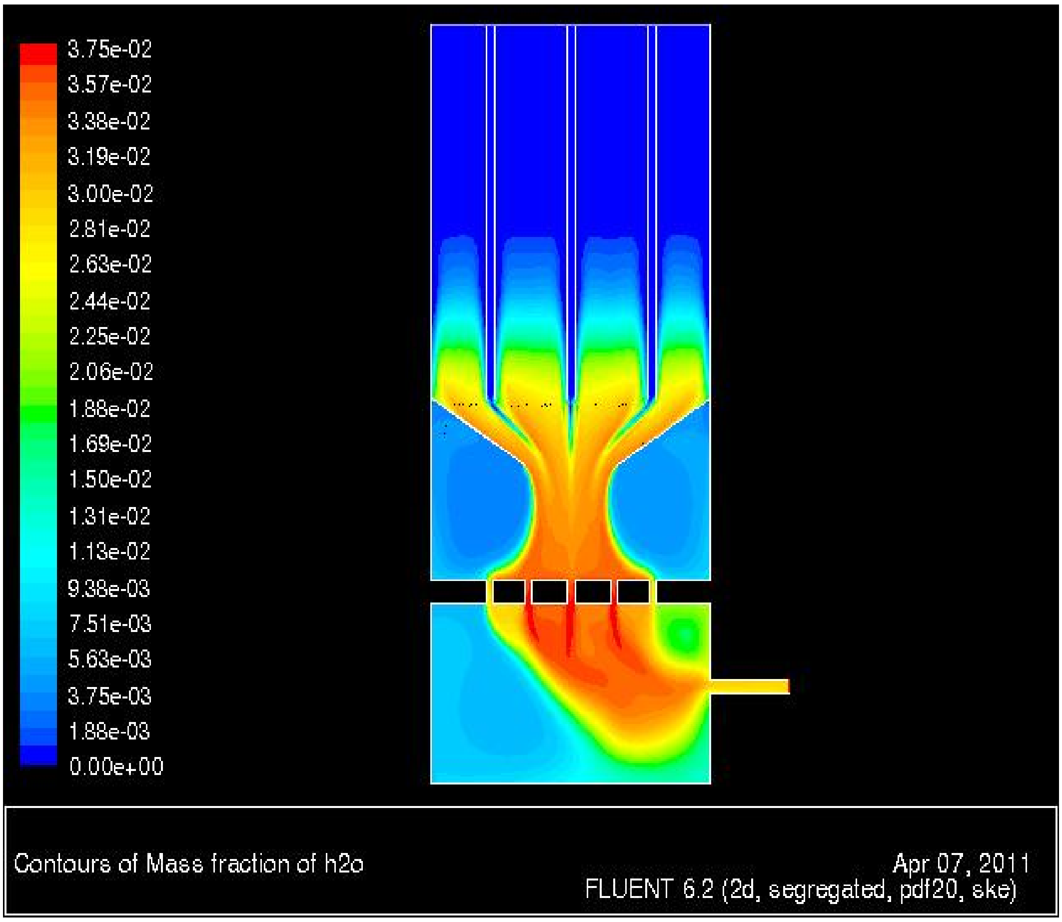

Figure 5.8: Mass fraction of H_2O

The very high H_2O mass fractions seen in the downstream of the gasifier near the exhaust nozzle.

5.9 Mass Fraction of H_2

The mass fraction of H_2 should increase at the gas nozzle part.But in the present case it is not obtained.The mass fraction in this case is 0.023 i.e 2.3%.This result might be deviated due to the uneven distribution of gas in the reaction chamber.

The mass fraction is high on a plane through inlets, as expected, but the highest mass fractions occur in the corners of the inlets where particles become trapped.This phenomenon is expected to be reduced when char reaction is taken in to account.

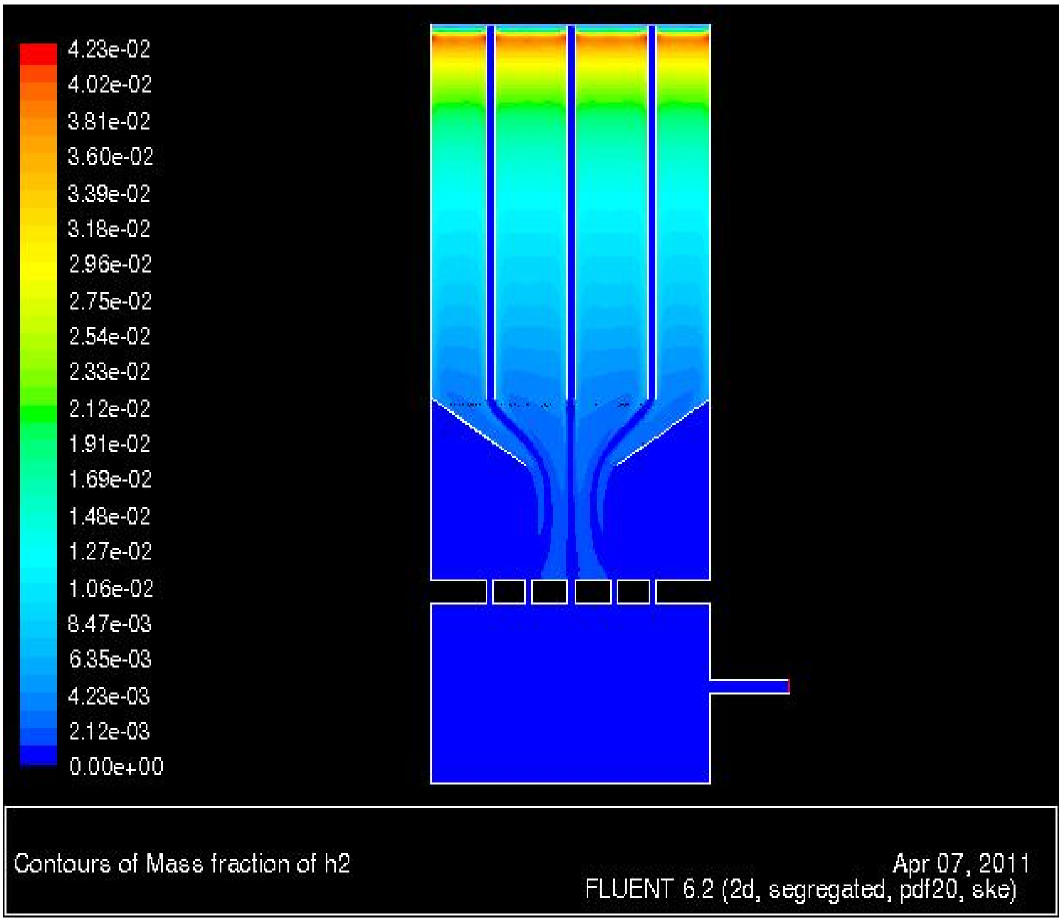

Figure 5.9: Mass fraction of H_2

5.10 Mass Fraction of O

There is only minor amount of oxygen in the coal portion. The reactive O molecules are found out below the grate region.This Oxygen redicals react with the CO and the final outcome from this two is CO_2 which is not desirable.More-or-less the O redicals are converted in to O_2 by heterogenous reactions which are taking place inside the pyrolysis zone.

At the exhaust nozzle, the concentration of O redicals is higher. The higher temperature below the grate portion also played major role in the result.

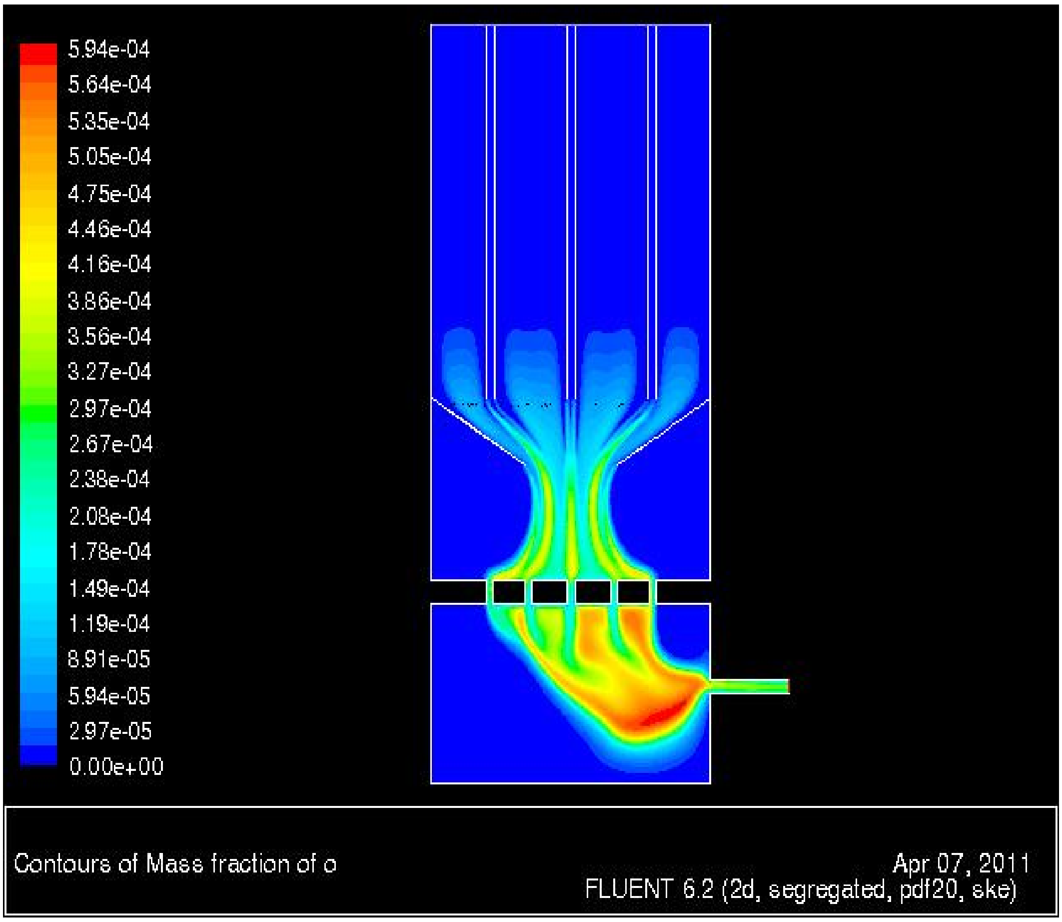

Figure 5.10: Mass fraction of O

Chapter 6

Conclusion and Future Scope

6.1 Conclusion

The model will be developed and would be used to predict the gas composition, reaction temperature, unconverted char and calorific value of gas for known coal composition, initial temperature of pyrolysis zone, velocity of air flow and pressure.

6.2 Future Scope

The current project enabled the basic understanding and formulation of 2d models for study of the gasification using CFD code. However more detailed models are required for extending these models to achieve results which can be applied into practical situations. The following list of possibilities is present for future work on this subject:

- Study of tar and tar modeling in a gasifier is also possible with the existing model,which is not performed in this dissertation.
- Construction of steady state models for pyrolysis and gasification zones will be done.Due to the time frame it is not possible to make a separate model for each zone.But it is possible to design a model for the zones.

- The computational fluid dynamics (CFD) software is playing a strong role as a design tool computer. Today CFD can be considered as an equal partner with pure theory and pure experiment in the analysis and solution of reactive as well as non-reactive systems. The development of new products of gasifier for coal is getting better if the trial and error methods are replaced with CFD software which can assist them in improving new products.

- The simulations still have many approximate models as well as some assumptions. To ensure CFD simulations are more than just theoretical exercises, experimental validation is necessary to facilitate the model accuracy. With the progressing of the computing power and the development of chemical and physical models, the CFD applications in the biomass thermochemical conversion will more widely spread in the future.

- There is consideration that has to put in mind about the environmental impact, from indirect and direct emissions release from the combustion process. For this dissertation, universal emission-releasing gas model based on coal is not evaluated although it is very necessary to analyze the product gas from the combustion process. This is because each case-dependent emissions associated with coal gasification practice is quite tedious and time-consuming.

- Thus, it is necessary in future to model the pollutants gas so that it can be used as reference when any gasifier are to be built on local community or society. So that they can be modeled based on simulation and can be evaluated in advance, as the result can be demonstrated from modeling using Computational Fluid Dynamics software.

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